

Compilation of Chemical Kinetic Data for Combustion Chemistry.

Part 1. Non-Aromatic C, H, O, N, and S Containing Compounds. (1971–1982)

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Foreword

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated physical and chemical property data. These tables are published in the *Journal of Physical and Chemical Reference Data*, in the NSRDS-NBS series of the National Bureau of Standards, and through other appropriate channels.

The task of critical evaluation is carried out in various data centers, each with a well-defined technical scope. A necessary preliminary step to the critical evaluation process is the retrieval from the world scientific literature of all papers falling within the scope of the center, followed by the extraction and organization of the numerical data contained in these papers. The present publication presents such a compilation of data prepared by the NBS Chemical Kinetics Data Center.

Further information on NSRDS and the publications which form the primary output of the program may be obtained by writing to the Office of Standard Reference Data, National Bureau of Standards, Gaithersburg, MD 20899.

DAVID R. LIDE, JR., *Director*
Office of Standard Reference Data

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Compilation of Chemical Kinetic Data for Combustion Chemistry. Part 1. Non-Aromatic C, H, O, N, and S Containing Compounds. (1971-1982)

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Chemical kinetics data for reactions of importance in combustion chemistry are compiled. Experimental, theoretical, evaluated, or estimated rate constants are given for reactions of O, O₂, O₃, H, H₂, OH, HO₂, H₂O, H₂O₂, N, N₂, N₃, NO, NO₂, NO₃, N₂O, N₂O₅, NH, NH₂, NH₃, NH=NH, NH₂=NH, NH₂=NH₂, HN₃, HNO, HONO, HONO₂, HO₂NO₂, NH₂O, NH₂O₂, S, S₂, SO, SO₂, SH, H₂S, and the aliphatic, alicyclic, and heterocyclic saturated and unsaturated C₁ to C₁₅ hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides, and their free radicals. The data were taken from the literature published between 1971 and 1982. Data previously issued in 1981 as NBSIR-81-2254, which covered the literature published from 1971 through 1977, are included. The data are reported as rate constants or in terms of the parameters *A*, *n*, and *B* of the extended Arrhenius expression $k = A(T/298)^n \times \exp(-B/T)$, where $B = E/R$. Data are given for 1931 reactions.

Key words: Arrhenius parameters; carbon; chemical kinetics; combustion; compilation; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur.

1. Introduction

1.1. Overview

This report provides a compilation of chemical kinetic data for use by modelers, experimentalists, and theoreticians interested in developing a detailed understanding of gas phase combustion processes involving fossil fuels. It is part of a larger effort to develop a comprehensive evaluated chemical kinetic data base, and is a necessary prelude to that effort. The present compilation covers the literature published between 1971 and 1982. It will be followed by subsequent compilations covering the literature published after 1982. These will then be updated approximately every three years.

The present work serves as the foundation for a set of evaluations on specific subsets of the larger data base. Those published or in preparation include:

- (1) "Chemical Kinetic Data Base for Combustion Chemistry. Part 1. Methane and Related Compounds", W. Tsang and R. F. Hampson, *J. Phys. Chem. Ref. Data* **15**, 1087 (1986).
- (2) "Chemical Kinetic Data Base for Combustion Chemistry. Part 2. Methanol", W. Tsang, *J. Phys. Chem. Ref. Data* **16**, (Sept. 1987).
- (3) "Chemical Kinetic Data Base for Combustion Chemistry. Part 3. Propane.", W. Tsang, *J. Phys. Chem. Ref. Data* (submitted).
- (4) "Chemical Kinetic Data Base for Combustion Chemistry. Part 4. Isobutane", W. Tsang (to be published).

- (5) "Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O(³P) with Unsaturated Hydrocarbons", R. J. Cvetanović, *J. Phys. Chem. Ref. Data* **16**, 261 (1987).
- (6) "Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O(³P) with Sulfur Containing Compounds", D. L. Singleton and R. J. Cvetanović (in preparation).
- (7) "Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O(³P) with Saturated Organic Compounds", John T. Herron, *J. Phys. Chem. Ref. Data* (submitted).

1.2. Scope

Data are given for the reactions of aliphatic, alicyclic, and heterocyclic, saturated and unsaturated hydrocarbons and their derivatives, and for the reactions with inorganic species containing hydrogen, oxygen, nitrogen, and sulfur with themselves and with hydrocarbons and their derivatives. Not included are reactions involving aromatic species, halogens, halogen derivatives, ions, and, with few exceptions, excited states.

The data have been abstracted from the literature published between 1971 and 1982 inclusive. Some references to earlier work are included. All data published earlier in NBSIR-81-2254¹ are included.

Only publications containing numerical data have been abstracted. The abstracted data are either rate constants at some given temperature or the parameters *A*, *n*, and *B* of the extended Arrhenius expression $k = A(T/298)^n \exp(-B/T)$. Additional data on temperature range, pressure, nature of the third body, and the type of data (i. e., experimental, theoretical, estimated, etc.) are also provided.

1.3. Guide to the Table

1.3.1. General

The compilation is divided into two parts — a table of rate constants and a bibliography, which contains the references to the cited literature. The following describes the arrangement of the table with respect to contents and the order in which reactions are listed.

1.3.2. Arrangement of the Table

The table is arranged in eight columns. These list the chemical reaction, the data type, the temperature, the rate constant or the Arrhenius A factor, the n factor, the B factor where $B = E/R$, a term indicating the appropriate units for the rate constants, and an error factor. Other necessary information (such as the bibliographic citation, pressure and nature of bath gas, and notes on methodology or other factors) is given in the same column as the chemical reaction. A detailed description follows:

(1) Column 1 gives the chemical reaction. The names of the reactants given are the Chemical Abstracts Standard Names. Synonyms, enclosed in parentheses, are in some cases also given. Product names are given only in those cases in which the product is a bridged compound.

The bibliographic citation is given in the form of a Reference Code, which consists of the last two digits of the year of publication, followed by the first three letters of the names of the first and second author (if present) separated by a slash. An integer index is attached at the end when it is necessary to differentiate between otherwise identical Codes. This is illustrated by the Code 82 ATK/ASC2.

This column may also include information on the experimental method, analytical procedures, nature of the third body, pressure, identity of reference reaction in the case of relative rate measurements, or other comments.

(2) Column 2 indicates the type of data. The following abbreviations are used:

- EX = experimental
- RL = relative rate measurement
- RN = relative rate measurement normalized to an absolute value
- TH = theoretical
- CO = computed numerically
- ES = estimated
- SE = selected value in the literature
- RE = current NBS recommended value.

(3) Column 3 gives the temperature or temperature range.

(4) Column 4 lists the rate constant or the Arrhenius A factor, or the ratio of the rate constants.

(5) Column 5 gives the factor n for the extended Arrhenius expression $k = A(T/298)^n \exp(-B/T)$.

(6) Column 6 gives the parameter B for the extended Arrhenius expression $k = A(T/298)^n \exp(-B/T)$, where B is the Arrhenius activation energy divided by the gas constant, i.e., $B = E/R$. In the case of relative rate measurements the quantity reported is the difference $B - B(\text{ref})$, where $B(\text{ref})$ is the value of B for the reference reaction.

(7) Column 7 indicates the units of the rate constant or the Arrhenius A factor.

(8) Column 8 gives the error factor as reported in the original work.

1.3.3. Order of Reactions

The reactions are listed following the order of arrangement given in Table 1 of "The NBS Tables of Thermodynamic Properties".² In the present compilation the reactants contain any of the elements O, H, S, N, and C, and the order used is: O system, H-O system, S-O-H system, N-O-H-S system, and C-O-H-S-N system. Examples of the ordering of reactant species are given below:

- (1) O system: O, O₂, O₃
- (2) H-O system: H, H₂, OH, HO₂, H₂O, H₂O₂
- (3) S-O-H system: S, S₂, SO, SO₂, SO₃, SH, H₂S
- (4) N-O-H-S system: N, N₂, NO₂, NO₃, N₂O, N₂O₃, NH, etc.
- (5) C-O-H-S-N system: C, CO, CO₂, CH, CH₂, CH₃, CH₄, etc.

Index of reactions given below in Sec. 3 follows the same order of arrangement and can be used to find the page where a particular reaction is located in the Table of Chemical Kinetic Data for Combustion Chemistry. The reaction of ethylene with oxygen atoms, for example, is located at its proper place in the "O ATOM Reactions" at the beginning of the Index, since O atom (the O system) precedes ethylene (the C system).

1.3.4. Chemical Formulas and Nomenclature

Where possible, chemical formulas are written in semi-structural form. The following conventions are used:

- (1) For C₁ through C₅ saturated hydrocarbons and their O, S, and N derivatives, semi-structural formulas are used, e.g., (CH₃)₂CH₂CH₂ONO. Beyond C₅ the condensed forms are used, e.g., CH₃(CH₂)₈CH₂CN.
- (2) Unsaturated compounds are written to show the position of the double or triple bond, e.g., CH₂=C=CH₂.
- (3) The structures of all alicyclic and heterocyclic compounds are specified with figures in the text.

1.4. Acknowledgments

This work was supported by the Department of Energy, Division of Basic Energy Sciences and the Office of Standard Reference Data of the National Bureau of Standards. The authors are especially indebted to Mrs. Geraldine Zumwalt and Ms. Rhoda Levin for their attention to many details in the keyboarding, editing and preparation of the manuscript.

1.5. References to the Introduction

¹F. Westley, "Tables of Experimental Rate Constants for Chemical Reactions Occurring in Combustion (1971-1977)", NBSIR 81-2254, National Bureau of Standards, Gaithersburg, MD 20899 (1981).

²D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, I. Halow, S. M. Bailey, K. L. Churney, and R. L. Nuttall, J. Phys. Chem. Ref. Data 11, Suppl. 2 (1982).

2. Summary of Symbols and Units

Data Type Codes:

- EX (experimentally measured absolute value),
- RL (experimentally measured relative value),
- RN (RL normalized to absolute value),
- TH (theoretical value),
- DE (derived indirectly, e.g. using reverse rate and equilibrium constant, or computer simulation of a complex mechanism)
- CO (computed numerically),
- ES (estimated, by analogy etc),
- SE (selected in the literature as probable "best" value),
- RE (currently recommended value).

Type of excitation:

- † (vibrationally excited)
- * (electronically excited)

Decadic exponent notation: 1.2(11) (stands for 1.2×10^{11})

Temperature (T): in kelvins (K).

Arrhenius parameters are defined by

$$k = A(T/298)^n \exp(-B/T)$$

Unit Codes for k , $k/k(\text{ref})$, A , $A/A(\text{ref})$:

- 1 (s^{-1}),
- 2 ($\text{cm}^3 \text{mol}^{-1} \text{s}^{-1}$),
- 3 ($\text{cm}^6 \text{mol}^{-2} \text{s}^{-1}$),
- 1/1, 2/2 etc. (dimensionless),
- 2/1 ($\text{cm}^3 \text{mol}^{-1}$), etc.

$(T/298)$ and n (the exponent of T) are dimensionless.

Units for B , $B-B(\text{ref})$: kelvins (K). (Activation energy $E = R \times B$).

$k(\text{ref})$, $A(\text{ref})$ and $B(\text{ref})$ are the values for the "reference reaction" in relative rate determinations.

k err. factor: Estimated overall Uncertainty Factor. It multiplies and divides k or A to indicate approximate error limits. It does not imply that errors in k are necessarily lognormally distributed.

3. Index of Reactions

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O + O ₂ (+ M)	51
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O(¹ D) + H ₂	58
O(¹ D) + D ₂	59
O + OH	59
O + HO ₂	60
O + H ₂ O	61
O(¹ D) + H ₂ O	61
O + H ₂ O ₂	63
O(¹ D) + H ₂ O ₂	63
O + SO (+ M)	63
O + SO ₂ (+ M)	63
O + SO ₃ (+ M)	64
O + S ₂ O	65
O + SH	65
O + H ₂ S	65
O + D ₂ S	66
O + N (+ M)	66
O + N ₂ (+ M)	66
O(¹ D) + N ₂ (+ M)	66
O + N ₃	67
O + NO (+ M)	67
O(¹ D) + NO	70
O + NO ₂ (+ M)	70
O(¹ D) + NO ₂	71
O + NO ₃	71
O + N ₂ O	71
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$O_2(^1\Delta_g)$ + $CH_3C(O)CH_2CH(CH_3)_2$ (2-Pentanone, 4-methyl-)	124
$O_2(^1\Delta_g)$ + $(CH_3)_2C=CHN(CH_3)_2$ (1-Propen-1-amine, N,N,2-trimethyl-)	124
$O_2(^1\Delta_g)$ + cy- $(CH_2)_4CH=C(CH_3)$ (Cyclohexene, 1-methyl-)	124
$O_2(^1\Delta_g)$ + cy- $(CH_2)_3C(CH_3)=C(CH_3)$ (Cyclopentene, 1,2-dimethyl-) ..	124
$O_2(^1\Delta_g)$ + $(CH_3)_2C=C(CH_3)CH_2CH_3$	125
O_2 + $CH_3(CH_2)_5CH_3$	125
$O_2(^1\Delta_g)$ + $CH_2=CHC(O)OCH_2CH_2CH_2CH_3$ (2-Propenoic acid butyl ester)	125
$O_2(^1\Delta_g)$ + $CH_3(CH_2)_5CHO$	125
$O_2(^1\Delta_g)$ + $CH_3C(O)OCH_2CH_2CH(CH_3)_2$ (1-Butanol, 3-methyl-, acetate)	125
O_2 + cy- $CH=CHCH=CHC(=CH_2)C(=CH_2)$ (1,3-Cyclohexadiene, 5,6-bis(methylene)-)	125
$O_2(^1\Delta_g)$ + cy- $(CH_2)_4C(CH_3)=C(CH_3)$ (Cyclohexene, 1,2-dimethyl-) ..	126
$O_2(^1\Delta_g)$ + $(CH_3)_2C=C(CH_3)CH_2CH_2CH_3$	126
O_2 + $(CH_3)_3CCH_2CH(CH_3)_2$ (Pentane, 2,2,4-trimethyl-)	126
$O_2(^1\Delta_g)$ + $C_2H_5OCH=C(C_2H_5)C_4H_9$ (1-Hexene, 1-ethoxy-2-ethyl-) ..	126

O_3 Reactions:

O_3 (+ M)	127
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$O_3 + SO$	127
$O_3(v=n) + SO$	127
$O_3 + SO_2$	128
$O_3 + H_2S$	128
$O_3 + NO$	128
$O_3 + NO^\dagger$	128
$O_3^\dagger + NO$	128
$O_3 + NO_2$	131
$O_3 + HONO$	131
$O_3 + CH_4$	132
$O_3 + HCHO$	132
$O_3 + CH_3ONO$	132
$O_3 + CH=CH$	132
$O_3 + CH_2=CH_2$	132
$O_3 + cis-CDH=CDH$	133
$O_3 + trans-CDH=CDH$	133
$O_3 + CD_2=CD_2$	133
$O_3 + CH_3CHO$	134
$O_3 + cy-CH_2CH_2S$ (Ethylene episulfide)	134
$O_3 + CH_3CH_2ONO$	134
$O_3 + CH_3C\equiv CH$	134
$O_3 + CH_2=C=CH_2$	134
$O_3 + CH_3CH=CH_2$	134
$O_3 + CD_3CD=CD_2$	135
$O_3 + CH_2=CHCHO$	135
$O_3 + CH_3C(O)CHO$	135
$O_3 + CH_2=CHCN$	135
$O_3 + CH_3CH_2C\equiv CH$	135
$O_3 + CH_3C\equiv CCH_3$	135
$O_3 + CH_2=CHCH=CH_2$	136
$O_3 + CH_3CH_2CH=CH_2$	136
$O_3 + CH_3CH=CHCH_3$	136
$O_3 + cis-CH_3CH=CHCH_3$	136
$O_3 + trans-CH_3CH=CHCH_3$	136
$O_3 + (CH_3)_2C=CH_2$	137
$O_3 + CH_3CH=CHCHO$	137
$O_3 + CH_3C(O)CH=CH_2$	137
$O_3 + CH_2=C(CH_3)CHO$	138
$O_3 + cy-CH=CHCH=CHS$ (Thiophene)	138
$O_3 + CH_2=C(CH_3)CH=CH_2$	138
$O_3 + cy-C_5H_8$ (Cyclopentene)	138
$O_3 + CH_3CH_2CH_2CH=CH_2$	138
$O_3 + cis-CH_3CH_2CH=CHCH_3$	138
$O_3 + trans-CH_3CH_2CH=CHCH_3$	139
$O_3 + CH_3CH=C(CH_3)_2$	139
$O_3 + CH_3C(O)CH=CHCH_3$	139
$O_3 + cy-CH=CH(CH_2)_4$ (Cyclohexene)	139
$O_3 + CH_3CH_2CH_2CH_2CH=CH_2$	139
$O_3 + CH_3CH_2CH_2C(CH_3)=CH_2$	140

O ₃ + (CH ₃) ₂ CHCH ₂ CH=CH ₂	140
O ₃ + cis-CH ₃ CH ₂ C(CH ₃)=CHCH ₃	140
O ₃ + trans-CH ₃ CH ₂ C(CH ₃)=CHCH ₃	140
O ₃ + (CH ₃) ₂ C=C(CH ₃) ₂	140
O ₃ + cy-C(O)CH=CH(CH ₂) ₃ (2-Cyclohexen-1-one)	140
O ₃ + CH ₃ (CH ₂) ₄ CH=CH ₂	140
O ₃ + cy-C ₁₀ H ₁₆ (Terpinolene)	141
O ₃ + bicy-C ₁₀ H ₁₆ (α-Pinene)	141
O ₃ + bicy-C ₁₀ H ₁₆ (β-Pinene)	141

H ATOM Reactions:

H + O ₂ (+ M)	142
H + O ₂ (¹ Δ _g)	144
D + O ₂ (+ M)	145
H + O ₃	145
H + H (+ M)	146
D + D (+ M)	147
H + H ₂ (v=1)	148
H + HD	148
H + HD(v=1)	148
H + D ₂	148
H + D ₂ (v=1)	148
D + H ₂	148
D + H ₂ (v=n)	149
D + HD	149
H + OH (+ M)	149
D + OH	149
H + OH + OH	150
H + OH + CO	150
H + HO ₂	150
H + H ₂ O	153
H + H ₂ O ₂	153
D + H ₂ O ₂	154
H + SO ₂	154
H + SH	154
H + H ₂ S	154
D + D ₂ S	155
H + N (+ M)	155
H + N ₂	155
H + NO (+ M)	155
D + NO (+ M)	157
H + NO ₂	157
H + N ₂ O	157
H + N ₂ O(v=3)	158
H + NH	158
H + NH ₂ (+ M)	158
H + NH ₃	159
H + NH ₂ NH	159

H + NH ₂ NH ₂	159
H + HN ₃	159
H + HNO	159
H + HONO ₂	160
H + HO ₂ NO ₂	160
H + CO (+ M)	160
H + CO + OH	160
H + CO ₂	161
H + CH	161
H + CH ₂	161
H + CH ₃ (+ M)	161
H + CH ₄	162
D + CD ₄	163
H + CHO	163
H + HCHO	164
H + CH ₃ O	164
H + CD ₃ O	165
D + CH ₃ O	165
H + CH ₂ OH	165
H + CD ₂ OH	165
D + CH ₂ OD	166
H + CH ₃ OH	166
H + CD ₃ OH	166
H + CD ₃ OD	167
D + CH ₃ OH	167
H + CH ₃ OOH	167
D + CH ₃ OOH	167
H + COS	167
H + CH ₂ =N=N	168
H + CH ₃ NO ₂	168
H + CH ₃ ONO	168
H + CD ₃ ONO	168
H + CH=CH (+ M)	168
H + CD=CD (+ M)	169
D + CH=CH	170
D + CD=CD	170
H + CH ₂ =CH	171
H + CH ₂ =CH ₂ (+ M)	171
H + CH ₂ =CHD	173
H + CD ₂ =CD ₂ (+ M)	173
D + CH ₂ =CH ₂	174
D + CH ₂ =CHD	174
D + CD ₂ =CD ₂	174
H + CH ₃ CH ₂	175
H + CH ₃ CH ₃	175
H + CH ₂ =C=O	175
H + CH ₃ CO	176
H + CH ₃ CHO	176
H + CH ₂ CH ₂ OH	176

H + CH ₃ CH ₂ OH	176
H + (CH ₃) ₂ O	176
D + (CH ₃) ₂ O	177
H + CH ₃ OOCH ₃	177
H + cy-CH ₂ CH ₂ S (Ethylene episulfide)	177
H + (CH ₃) ₂ S	177
H + CH ₃ SSCH ₃	178
H + NCCN	178
H + O=C=C=C=O	178
H + CH ₃ C=CH	178
H + CH ₂ =C=CH ₂	178
H + CH ₃ CH=CH ₂	179
H + CD ₃ CD=CD ₂	181
D + CH ₃ CH=CH ₂	181
D + CD ₃ CD=CD ₂	181
H + (CH ₃) ₂ CH	181
H + (CH ₃) ₂ CH [†]	182
H + CH ₃ CH ₂ CH ₃	182
H + CH ₂ =CHCHO	182
H + (CH ₃) ₂ CO	182
H + CH=CC=CH	183
H + CH ₂ =CHC=CH	183
H + CH ₂ =CHCH=CH ₂ (+ M)	183
D + CH ₂ =CHCH=CH ₂	183
H + CH ₃ CH ₂ CH=CH ₂	184
D + CH ₃ CH ₂ CH=CH ₂	185
H + CH ₃ CH=CHCH ₃ (unspecified form)	185
H + cis-CH ₃ CH=CHCH ₃	185
D + cis-CH ₃ CH=CHCH ₃	186
H + trans-CH ₃ CH=CHCH ₃	186
D + trans-CH ₃ CH=CHCH ₃	187
H + (CH ₃) ₂ C=CH ₂ (+ M)	187
D + (CH ₃) ₂ C=CH ₂	188
H + (CH ₃) ₃ C	188
H + (CH ₃) ₃ C [†]	189
H + CH ₃ CH ₂ CH ₂ CH ₃	189
H + (CH ₃) ₃ CH	189
H + (CH ₃) ₃ COH	190
H + (CH ₃ CH ₂) ₂ O	190
H + cy-CH ₂ CH ₂ CH ₂ CH ₂ S (Thiophene, tetrahydro-)	190
H + CH ₃ CH ₂ CH ₂ CH ₂ SH	190
H + (CH ₃ CH ₂) ₂ S	190
H + CH ₃ CH ₂ SSCH ₂ CH ₃	191
H + CH ₃ CH ₂ CH ₂ CH=CH ₂	191
H + CH ₃ CH ₂ CH=CHCH ₃ (unspecified form)	191
H + CH ₃ CH ₂ C(CH ₃)=CH ₂	192
D + CH ₃ CH ₂ C(CH ₃)=CH ₂	192
H + (CH ₃) ₂ CHCH=CH ₂	192
D + (CH ₃) ₂ CHCH=CH ₂	192

H + CH ₃ CH=C(CH ₃) ₂	192
D + CH ₃ CH=C(CH ₃) ₂	193
H + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃	193
H + (CH ₃) ₂ CHCH ₂ CH ₃	193
H + (CH ₃) ₄ C	193
H + (CH ₃) ₃ COCH ₃	194
H + CH ₃ CH ₂ CH ₂ C(CH ₃)=CH ₂	194
H + CH ₃ CH ₂ CH=C(CH ₃) ₂	194
H + CH ₃ CH ₂ C(CH ₃)=CHCH ₃	194
H + (CH ₃) ₂ C=C(CH ₃) ₂	195
D + (CH ₃) ₂ C=C(CH ₃) ₂	195
D + cy-C ₆ H ₁₂ (Cyclohexane)	195
H + CH ₃ (CH ₂) ₄ CH ₃	195
H + (CH ₃) ₂ CHCH(CH ₃) ₂	195
H + (CH ₃) ₂ CHN=NCH(CH ₃) ₂	196
H + (CH ₃) ₃ CCH(CH ₃) ₂	196
H + (CH ₃) ₃ CC(CH ₃) ₃	196

H₂ Reactions:

H ₂ (+ M)	197
D ₂ (+ M)	197
H ₂ + D ₂	197
HD + HD	197
H ₂ + NO	197
H ₂ (v>5) + NO	198
H ₂ + NO ₂	198
H ₂ + N ₂ O	198
H ₂ (X ¹ Σ _g ⁺) + C ₂ (X ¹ Σ _g ⁺)	198
H ₂ (X ¹ Σ _g ⁺) + C ₂ (a ³ Π _u)	199
D ₂ + C ₂ (a ³ Π _u)	199
H ₂ + C ₂ O	199
D ₂ + CH=CH	199
H ₂ + C ₃	199
H ₂ + cy-CH ₂ CH ₂ CH=CHCH=CH (1,3-Cyclohexadiene)	199

OH RADICAL Reactions:

OH + O ₃	200
OH(v=n) + O ₃	200
OD(v=n) + O ₃	200
OH + H ₂	201
OH(v=1) + H ₂	202
OH(v=n) + H ₂ (v=1)	202
OH + HD	203
OH + D ₂	203
OD + H ₂	203
OD + D ₂	204
OH + OH (+ M)	204

OH + HO ₂	205
OH(v=9) + H ₂ O	207
OH + H ₂ O ₂	207
OH + S	208
OH + SO	208
OH + SO ₂ (+ M)	209
OH(v=9) + SO ₂	210
OH + H ₂ S	211
OH(v=9) + H ₂ S	211
OH + N ₂	212
OH(v=9) + N ₂	212
OH + NO (+ M)	212
OH(v=9) + NO	214
OH + NO ₂ (+ M)	214
OH + N ₂ O (+ M)	218
OH(v=9) + N ₂ O	218
OH + NH ₂	218
OH + NH ₃	219
OH + NH ₂ NH ₂	220
OH + HNO	220
OH + HONO	220
OH + HONO ₂	220
OH + HO ₂ NO ₂	222
OH + CO	222
OH + CO [†]	226
OD + CO	226
OH(v=1) + CO	227
OH(v=9) + CO ₂	227
OH + CH ₃	227
OH + CH ₄	228
OH(v=n) + CH ₄	229
OH + CDH ₃	229
OH + CD ₂ H ₂	229
OH + CD ₃ H	229
OH + CD ₄	230
OH + HCHO	230
OH + HCOOH	231
OH + CH ₃ OH	231
OH + CS ₂	231
OH + COS	232
OH(v=9) + COS	233
OH + CH ₃ SH	233
OH + CN	233
OH + HCN	234
OH + CH ₃ NH ₂	234
OH + NH ₂ NHCH ₃	234
OH + CH ₃ ONO	234
OH + CH ₃ NO ₂	234
OH + CH=CH	235

OH + CH ₂ =CH ₂	236
OH + CD ₂ =CD ₂	238
OH + CH ₃ CH ₃	238
OH + CH ₂ =C=O	239
OH + CH ₃ CHO	239
OH + CH ₃ COOH	239
OH + CH ₃ CH ₂ OH	239
OH + (CH ₃) ₂ O	240
OH + (CH ₃) ₂ S	240
OH + CH ₃ SSCH ₃	240
OH + NCCN	241
OH + CH ₃ CN	241
OH + CH ₃ N=NCH ₃	241
OH + CH ₃ CH ₂ NH ₂	241
OH + (CH ₃) ₂ NH	241
OH + CH ₃ C(O)O ₂ NO ₂ (Peroxide, acetyl nitro-)	241
OH + CH ₃ CH ₂ ONO	242
OH + O=C=C=C=O	242
OH + CH ₃ C≡CH	242
OH + CH ₂ =C=CH ₂	242
OH + CH ₃ CH=CH ₂	242
OH + CD ₃ CH=CH ₂	244
OH + CH ₃ CD=CD ₂	244
OH + CD ₃ CD=CD ₂	244
OH + CH ₃ CH ₂ CH ₃	245
OH + CH ₂ =CHCHO	246
OH + CH ₃ C(O)CHO	246
OH + CH ₂ =CHCH ₂ OH	246
OH + CH ₂ =CHOCH ₃	247
OH + CH ₃ CH ₂ CHO	247
OH + (CH ₃) ₂ CO	247
OH + CH ₃ CH ₂ COOH	248
OH + CH ₃ C(O)OCH ₃	248
OH + CH ₃ CH ₂ CH ₂ OH	248
OH + (CH ₃) ₂ CHOH	248
OH + CH ₂ =CHCN	248
OH + CH ₃ CH ₂ CN	248
OH + (CH ₃) ₃ N	249
OH + CH ₃ CH ₂ CH ₂ ONO	249
OH + (CH ₃) ₂ CHONO ₂	249
OH + CH=CC=CH	249
OH + CH ₂ =CHCH=CH ₂	249
OH + CH ₃ CH ₂ CH=CH ₂	250
OH + cis-CH ₃ CH=CHCH ₃	250
OH + trans-CH ₃ CH=CHCH ₃	251
OH + (CH ₃) ₂ C=CH ₂	252
OH + cy-C ₄ H ₈ (Cyclobutane)	252
OH + CH ₃ CH ₂ CH ₂ CH ₃	252

OH + CD ₃ CD ₂ CD ₂ CD ₃	254
OD + CH ₃ CH ₂ CH ₂ CH ₃	254
OD + CD ₃ CD ₂ CD ₂ CD ₃	254
OH + (CH ₃) ₃ CH	254
OH + cy-CH=CHCH=CHO (Furan)	256
OH + CH ₃ CH=CHCHO	256
OH + CH ₃ C(O)CH=CH ₂	256
OH + CH ₂ =C(CH ₃)CHO	256
OH + CH ₃ CH ₂ CH ₂ CHO	256
OH + (CH ₃) ₂ CHCHO	257
OH + CH ₃ C(O)CH ₂ CH ₃	257
OH + CH ₃ CH ₂ CH ₂ COOH	258
OH + CH ₃ C(O)OCH ₂ CH ₃	258
OH + CH ₃ CH ₂ C(O)OCH ₃	258
OH + cy-CH ₂ CH ₂ CH ₂ CH ₂ O (Furan, tetrahydro-)	258
OH + CH ₃ CH ₂ CH ₂ CH ₂ OH	258
OH + (CH ₃ CH ₂) ₂ O	259
OH + (CH ₃) ₃ COOH	259
OH + cy-CH=CHCH=CHS (Thiophene)	259
OH + CH ₃ CH ₂ CH ₂ CH ₂ ONO	259
OH + CH ₃ CH ₂ CH(CH ₃)ONO	259
OH + (CH ₃) ₂ CHCH ₂ ONO	260
OH + (CH ₃) ₃ CONO	260
OH + CH ₃ CH ₂ CH ₂ CH ₂ ONO ₂	260
OH + CH ₃ CH ₂ CH(CH ₃)ONO ₂	260
OH + (CH ₃ CH ₂) ₂ NOH	261
OH + CH ₂ =C(CH ₃)CH=CH ₂	261
OH + CH ₃ CH ₂ CH ₂ CH=CH ₂	261
OH + CH ₃ CH ₂ CH=CHCH ₃	262
OH + cis-CH ₃ CH ₂ CH=CHCH ₃	262
OH + CH ₃ CH ₂ C(CH ₃)=CH ₂	262
OH + (CH ₃) ₂ CHCH=CH ₂	262
OH + (CH ₃) ₂ C=CHCH ₃	262
OH + cy-C ₅ H ₁₀ (Cyclopentane)	263
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃	263
OH + (CH ₃) ₂ CHCH ₂ CH ₃	264
OH + (CH ₃) ₄ C	265
OH + CH ₃ CH ₂ CH ₂ CH ₂ CHO	265
OH + (CH ₃) ₂ CHCH ₂ CHO	266
OH + (CH ₃) ₃ CCHO	266
OH + CH ₃ C(O)CH ₂ CH ₂ CH ₃	267
OH + (CH ₃ CH ₂) ₂ CO	267
OH + CH ₃ C(O)OCH ₂ CH ₂ CH ₃ (Acetic acid propyl ester)	267
OH + CH ₃ CH ₂ C(O)OCH ₂ CH ₃ (Propanoic acid ethyl ester)	267
OH + CH ₃ CH ₂ CH ₂ CH(CH ₃)ONO ₂ (2-Pentanol nitrate)	267
OH + (CH ₃ CH ₂) ₂ CHONO ₂ (3-Pentanol nitrate)	268
OH + cy-(CH ₂) ₄ CH=CH (Cyclohexene)	268
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Hexene)	268

OH + (CH ₃) ₃ CCH=CH ₂ (1-Butene, 3,3-dimethyl-)	268
OH + (CH ₃) ₂ C=C(CH ₃) ₂	269
OH + cy-C ₆ H ₁₂ (Cyclohexane)	269
OH + n-C ₆ H ₁₄	269
OH + (CH ₃) ₂ CHCH ₂ CH ₂ CH ₃ (Pentane, 2-methyl-)	270
OH + CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₃ (Pentane, 3-methyl-)	270
OH + (CH ₃) ₂ CHCH(CH ₃) ₂	271
OH + CH ₃ C(O)CH ₂ CH ₂ CH ₂ CH ₃ (2-Hexanone)	271
OH + CH ₃ CH ₂ C(O)CH ₂ CH ₂ CH ₃ (3-Hexanone)	272
OH + CH ₃ C(O)CH ₂ CH(CH ₃) ₂ (2-Pentanone, 4-methyl-)	272
OH + CH ₃ C(O)OCH(CH ₃)CH ₂ CH ₃ (Acetic acid 1-methylpropyl ester)	272
OH + CH ₃ CH ₂ CH ₂ OCH ₂ CH ₂ CH ₃ (di-n-Propyl ether)	273
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH(CH ₃)ONO ₂ (2-Hexanol nitrate)	273
OH + CH ₃ CH ₂ CH ₂ CH(CH ₂ CH ₃)ONO ₂ (3-Hexanol nitrate)	273
OH + cy-(CH ₂) ₄ CH=C(CH ₃) (Cyclohexene, 1-methyl-)	273
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Heptene)	273
OH + n-C ₇ H ₁₆ (n-Heptane)	274
OH + (CH ₃) ₃ CCH(CH ₃) ₂ (Butane, 2,2,3-trimethyl-)	274
OH + (CH ₃) ₂ CHC(O)CH(CH ₃) ₂ (3-Pentanone, 2,4-dimethyl-)	275
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH(CH ₂ CH ₃)ONO ₂ (3-Heptanol nitrate)	275
OH + n-C ₈ H ₁₈ (n-Octane)	275
OH + CH ₃ (CH ₂) ₄ CH(CH ₂ CH ₃)ONO ₂ (3-Octanol nitrate)	275
OH + n-C ₉ H ₂₀ (n-Nonane)	276
OH + (CH ₃) ₂ CHCH ₂ C(O)CHCH ₂ (CH ₃) ₂ (4-Heptanone, 2,6-dimethyl-)	276
OH + bicy-C ₁₀ H ₁₆ (α-Pinene)	276
OH + bicy-C ₁₀ H ₁₆ (β-Pinene)	277
OH + n-C ₁₀ H ₂₂ (n-Decane)	277

HO₂ RADICAL Reactions:

HO ₂ + O ₃	277
HO ₂ + HO ₂ (+ M)	277
DO ₂ + DO ₂	280
HO ₂ + SO ₂ (+ M)	280
HO ₂ + NO (+ M)	280
DO ₂ + NO	282
HO ₂ + NO ₂ (+ M)	282
HO ₂ + N ₂ O	284
HO ₂ + NH ₂	284
HO ₂ + CO (+ M)	284
HO ₂ + CH ₄	285
HO ₂ + HCHO	285
HO ₂ + CH ₃ O ₂	286
HO ₂ + CH ₃ OH	286
HO ₂ + CH ₂ =CH ₂	286
HO ₂ + CH ₃ CH ₃	287
HO ₂ + CH ₃ CHO	287
HO ₂ + CH ₂ CH ₂ OH	287
HO ₂ + CH ₃ CH=CH ₂	287

HO ₂ + CH ₃ CH ₂ CH ₃	287
HO ₂ + CH ₃ CH ₂ CHO	288
HO ₂ + trans-CH ₃ CH=CHCH ₃	288
HO ₂ + (CH ₃) ₃ CH	288
HO ₂ + CH ₃ CH ₂ CH ₂ CHO	289
HO ₂ + (CH ₃) ₂ CHCHO	289
HO ₂ + (CH ₃) ₂ C=C(CH ₃) ₂	289
HO ₂ + (CH ₃) ₂ CHCH(CH ₃) ₂ (Butane, 2,3-dimethyl-)	289

H₂O Reactions:

H ₂ O (+ M)	289
D ₂ O (+ M)	290
H ₂ O + SO ₃	290
H ₂ O + NO ₂	290
H ₂ O + NO ₂ + NO ₂	290
H ₂ O + N ₂ O ₃	290
H ₂ O + N ₂ O ₄	290
H ₂ O + N ₂ O ₅	291

H₂O₂ Reactions:

H ₂ O ₂ (+ M)	291
H ₂ O ₂ + NO	291
H ₂ O ₂ + NO ₂	291
H ₂ O ₂ + N ₂ O ₅	291
H ₂ O ₂ + HONO ₂	291

S_x ATOM Reactions:

S + O ₂	292
S + O ₃	292
S(¹ D) + H ₂	292
S + S (+ M)	292
S + SH	292
S(¹ D) + N ₂	292
S(¹ D) + NO	292
S + NO (+ M)	293
S + NO ₂	293
S(¹ D) + N ₂ O	293
S(¹ D) + CO	293
S(¹ D) + CO ₂	293
S(¹ D) + CH ₄	293
S + COS	294
S(¹ D) + COS	294
S + CH=CH	294
S(¹ D) + CH=CH	295
S + CD=CD	295
S + CH ₂ =CH ₂	295

S + CH ₂ =CD ₂	295
S + cis-CHD=CHD	296
S + CD ₂ =CD ₂	296
S(¹ D) + CH ₂ =CH ₂	296
S(¹ D) + CH ₃ CH ₃	296
S + cy-CH ₂ CH ₂ S (Ethylene episulfide)	296
S + CH ₃ C=CH	297
S + CH ₃ CH=CH ₂	297
S + cy-CH(CH ₃)CH ₂ S (Thiirane, methyl-)	297
S + CH ₃ CH ₂ C≡CH	297
S + CH ₃ C≡CCH ₃	298
S + CH ₂ =CHCH=CH ₂	298
S + CH ₃ CH ₂ CH=CH ₂	298
S + cis-CH ₃ CH=CHCH ₃	299
S + trans-CH ₃ CH=CHCH ₃	299
S + (CH ₃) ₂ C=CH ₂	299
S + CH ₃ CH ₂ C≡CCH ₃	300
S + cy-C ₅ H ₈ (Cyclopentene)	300
S + CH ₃ CH ₂ C(CH ₃)=CH ₂	300
S + (CH ₃) ₂ C=CHCH ₃	300
S + (CH ₃) ₂ C=C(CH ₃) ₂	300
S ₂ (+ M)	301
S ₂ + S ₂ (+ M)	301

SO_x-COMPOUND Reactions:

SO (+ M)	301
SO + O ₂	301
SO + SO (+ M)	302
SO + SO ₃	302
SO + (SO) ₂ (Sulfur monoxide dimer)	302
SO + NO ₂	302
SO ₂ (+ M)	302
SO ₂ + SO ₂ (¹ B ₁)	303
SO ₂ + SO ₂ (³ B ₁)	303
SO ₂ + NO ₂	303
SO ₂ + NO ₃	304
SO ₂ + N ₂ O ₅	304
SO ₂ + CO	304
SO ₂ [*] + CO	304
SO ₂ ^{**} + CO	304
SO ₂ + CH=CH	305
SO ₂ (³ B ₁) + CH≡CH	305
SO ₂ (³ B ₁) + cis-CH ₃ CH=CHCH ₃	305
SO ₂ (³ B ₁) + trans-CH ₃ CH=CHCH ₃	305
SO ₂ (¹ B ₁) + (CH ₃) ₃ CH	305
SO ₂ (³ B ₁) + (CH ₃) ₃ CH	305
SO ₂ (³ B ₁) + cis-CH ₃ CH ₂ CH=CHCH ₃	305
SO ₂ (³ B ₁) + trans-CH ₃ CH ₂ CH=CHCH ₃	306

SO ₃ (+ M)	306
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SH_x-COMPOUND Reactions:

SH + D ₂	306
SH + SH	306
SH + NO	306
H ₂ S (+ M)	306

N_x-COMPOUND Reactions:

N(4S) + O ₂	307
N(2D) + O ₂	307
N(2P) + O ₂	307
N + O ₂ (¹ Δ _g)	307
N + O ₃	308
N(2D) + O ₃	308
N(2D) + H ₂	308
N + H ₂ (+ M)	308
N + OH	308
N(2D) + H ₂ O	309
N + SO ₃	309
N + N (+ M)	309
N + NO	309
N(2D) + NO	310
N(2P) + NO	310
N + NO ₂	310
N(2D) + N ₂ O	310
N(2P) + N ₂ O	311
N + HN ₃ (Hydrazoic acid)	311
N + NH ₂ NH ₂	311
N + C (+ M)	311
N(2D) + CO ₂	311
N + HCHO	311
N + CH ₃ OH	311
N + CH ₃ OD	312
N + CN	312
N + CH=CH	312
N + CH ₂ =CH ₂ (+ M)	312
N(2D) + CH ₂ =CH ₂	312
N(2P) + CH ₂ =CH ₂	313
N + CH ₃ CH ₂ OH	313
N + CH ₃ C=CH	313
N + CH ₃ CH=CH ₂	313
N + CH ₃ CH ₂ CH ₂ OH	313
N + (CH ₃) ₂ CHOH	313
N + CH ₂ =CHCH=CH ₂	314
N + CH ₃ CH ₂ CH=CH ₂	314
N + cis-CH ₃ CH=CHCH ₃	314

N + trans-CH ₃ CH=CHCH ₃	314
N + (CH ₃) ₂ C=CH ₂	314
N + NCC=CCN (2-Butynedinitrile)	314
N + (CH ₃) ₂ C=CHCH ₃	314
N ₂ (+ M)	315
N ₂ (A ³ Σ _u ⁺) + O ₂	315
N ₂ (A ³ Σ _u ⁺ , v=n) + O ₂	315
N ₃ + N ₃	315

N_xO_y-COMPOUND Reactions:

NO (+ M)	316
NO + O ₂ (¹ Δ _g)	316
NO + NO	316
NO + NO + NO	316
NO + NO + O ₂	316
NO + NO ₂ + H ₂ O	317
NO + NO ₃	317
NO + N ₂ O	317
NO + NH ₂	317
NO + NH ₃	317
NO + HNO	318
NO + HONO ₂	318
NO + C ₂ O	318
NO ₂ (+ M)	318
NO ₂ + NO ₂	318
NO ₂ + NO ₂ + CH ₃ OH	318
NO ₂ + NO ₂ + cy-CH ₂ CH ₂ O (Ethylene epoxide)	319
NO ₂ + NO ₂ + CH ₃ CH ₂ OH	319
NO ₂ + NO ₃ (+ M)	319
NO ₂ + NH ₃	320
NO ₂ + HONO	320
NO ₂ + CH ₄	320
NO ₂ + HCN	320
NO ₂ + CH ₂ =CH ₂	320
NO ₂ + CH ₃ CHO	320
NO ₂ + CH ₃ C=CH	321
NO ₂ + CH ₃ CH=CH ₂	321
NO ₂ + CH ₃ CH ₂ CH ₃	321
NO ₂ + CH ₃ CH ₂ CHO	321
NO ₂ + (CH ₃) ₂ CO	321
NO ₂ + CH ₂ =CHC=CH	321
NO ₂ + CH ₃ C=CCH ₃	321
NO ₂ + CH ₃ CH ₂ CH=CH ₂	321
NO ₂ + cis-CH ₃ CH=CHCH ₃	321
NO ₂ + trans-CH ₃ CH=CHCH ₃	322
NO ₂ + (CH ₃) ₂ C=CH ₂	322
NO ₂ + CH ₃ CH ₂ CH ₂ CHO	322
NO ₂ + CH ₃ CH ₂ N(↑O)=CHCH ₃ (Ethanamine, N-ethylidene-N-oxide-) ..	322

$\text{NO}_2 + (\text{CH}_3\text{CH}_2)_2\text{NOH}$ (Ethanamine, N-ethyl-N-hydroxy-)	322
$\text{NO}_2 + \text{CH}_2=\text{CHC}(\text{CH}_3)=\text{CH}_2$	322
$\text{NO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$	323
$\text{NO}_3 + \text{NO}_3$	323
$\text{NO}_3 + \text{CH}_2=\text{CH}_2$	323
$\text{NO}_3 + \text{CH}_3\text{CHO}$	323
$\text{NO}_3 + \text{CH}_3\text{CH}=\text{CH}_2$	323
$\text{NO}_3 + \text{CD}_3\text{CD}=\text{CD}_2$	323
$\text{NO}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$	324
$\text{NO}_3 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$	324
$\text{NO}_3 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	324
$\text{NO}_3 + (\text{CH}_3)_2\text{C}=\text{CH}_2$	324
$\text{NO}_3 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2$	324
$\text{NO}_3 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	324
$\text{N}_2\text{O} (+ \text{M})$	324
$\text{N}_2\text{O}_5 (+ \text{M})$	326

N_xH_y -COMPOUND Reactions:

$\text{NH} + \text{O}_2$	327
$\text{NH} + \text{H}_2$	327
$\text{NH} + \text{N}_2 (+ \text{M})$	327
$\text{NH} + \text{NO}$	327
$\text{NH} + \text{NH}_2$	328
$\text{NH} + \text{NH}_3 (+ \text{M})$	328
$\text{NH}(a^1\Delta) + \text{HN}_3(1A')$	328
$\text{NH}(b^1\Sigma^+) + \text{NH}_3$	328
$\text{NH}(a^1\Delta) + \text{CH}_4$	329
$\text{NH}(a^1\Delta) + \text{CH}_2=\text{CH}_2$	329
$\text{NH}(a^1\Delta) + \text{cy-C}_3\text{H}_6$ (Cyclopropane)	329
$\text{NH}(a^1\Delta) + \text{cy-C}_6\text{H}_{12}$ (Cyclohexane)	329
$\text{NH}_2 + \text{O}_2 (+ \text{M})$	329
$\text{NH}_2 + \text{O}_3$	330
$\text{NH}_2 + \text{H}_2$	330
$\text{NH}_2 + \text{NO}$	331
$\text{NH}_2 + \text{NO}_2$	332
$\text{NH}_2 + \text{NH}_2 (+ \text{M})$	333
$\text{NH}_2 + \text{NH}_2\text{NH}_2$	333
$\text{NH}_2(2A_1) + \text{HN}_3(1A')$	334
$\text{NH}_2(2A_1) + \text{CH}_4$	334
$\text{NH}_2 + \text{HCONH}_2$ (Formamide)	334
$\text{NH}_2 + \text{CH}=\text{CH}$	334
$\text{NH}_2 + \text{CH}_2=\text{CH}_2$	334
$\text{NH}_2(2A_1) + \text{CH}_2=\text{CH}_2$	335
$\text{NH}_2 + \text{CH}_3\text{CH}_2$	335
$\text{NH}_2 + \text{CH}_3\text{CH}_3$	335
$\text{NH}_2 + \text{CH}_2=\text{C}=\text{CH}_2$	335
$\text{NH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$	335
$\text{NH}_2 + \text{cy-C}_3\text{H}_6$ (Cyclopropane)	336

$\text{NH}_2(^2\text{A}_1) + \text{cy-C}_3\text{H}_6$ (Cyclopropane)	336
$\text{NH}_2 + (\text{CH}_3)_2\text{CH}$	336
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_3$	336
$\text{NH}_2 + \text{CH}_2=\text{CHCH}=\text{CH}_2$	337
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$	337
$\text{NH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$	337
$\text{NH}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	337
$\text{NH}_2 + (\text{CH}_3)\text{C}=\text{CH}_2$	337
$\text{NH}_2 + (\text{CH}_3)_3\text{C}$	337
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	338
$\text{NH}_2 + (\text{CH}_3)_3\text{CH}$	338
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	338
$\text{NH}_3 (+ \text{M})$	338
$\text{NH}_3 + \text{HONO}$	339
$\text{NH}_3 + \text{CH}_2=\text{CHCN}$	339
$\text{NH}=\text{NH}$ (Diazene)	340
$\text{cis-NH}=\text{NH} + \text{CH}_2=\text{CHCH}=\text{CH}_2$	340
$\text{cis-NH}=\text{NH} + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$	340
$\text{cis-NH}=\text{NH} + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	340
$\text{cis-NH}=\text{NH} + \text{cy-CH}_2\text{CH}_2\text{CH}=\text{CHCH}=\text{CH}$ (1,3-Cyclohexadiene)	340
$\text{cis-NH}=\text{NH} + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	340
$\text{trans-NH}=\text{NH}$	341
$\text{trans-NH}=\text{NH} + \text{cis-NH}=\text{NH}$	341
$\text{trans-ND}=\text{ND}$	341
$\text{trans-ND}=\text{ND} + \text{cis-ND}=\text{ND}$	341
$\text{NH}_2\text{NH} + \text{NH}_2\text{NH}$	341
$\text{NH}_2\text{NH}_2 (+ \text{M})$	341
$\text{HN}_3 (+ \text{M})$	341

NH_xO_y -COMPOUND Reactions:

$\text{HNO} + \text{HNO}$	342
$\text{DNO} + \text{DNO}$	342
$\text{HONO} (+ \text{M})$	342
$\text{HONO}\dagger$	342
$\text{HONO} + \text{O}_3$	343
$\text{HONO} + \text{HONO}$	343
$\text{HONO} + \text{HONO}_2$	343
$\text{HONO}_2 (+ \text{M})$	343
$\text{HO}_2\text{NO}_2 (+ \text{M})$	344
NH_2O	344
$\text{NH}_2\text{O} + \text{O}_3$	344
$\text{NH}_2\text{O}_2\dagger$ (Aminodioxy)	344

C ATOM Reactions:

$\text{C} + \text{O}_2$	345
$\text{C}(2^1\text{D}_2) (+ \text{M})$	345
$\text{C}(2^1\text{D}_2) + \text{H}_2$	345

C + H ₂ (+ M)	345
C + H ₂ O	345
C + N ₂ (+ M)	345
C + NO	346
C + N ₂ O	346
C + C (+ M)	346
C + CO (+ M)	346
C + CO ₂	346
C + CH ₂	346
C + CH ₄	347
C + CN	347
C + O=C=C=C=O	347
C(¹ S ₀) + O=C=C=C=O	347

CO_x-COMPOUND Reactions:

CO + O ₂	347
CO + O ₃	347
CO + SO ₂ (³ B ₁)	347
CO + NO ₂	347
CO + NO ₂ (² B ₂)	348
CO + N ₂ O	348
CO ₂ (+ M)	348
CO ₂ + C ₂ O	349

CH RADICAL Reactions:

CH + O ₂	349
CH + H ₂	349
CH + H ₂ O	350
CH + N ₂ (+ M)	350
CH + NO	350
CH + NO ₂	351
CH + N ₂ O	351
CH + NH ₃	351
CH + CO	351
CH + CO ₂	352
CH + CH ₂	352
CH + CH ₄	352
CH + CH=CH	352
CH + CH ₂ =CH ₂	353
CH + CH ₃ CH ₃	353
CH + CH ₃ C=CH	354
CH + cy-C ₃ H ₆ (Cyclopropane)	354
CH + CH ₃ CH ₂ CH ₃	354
CH + CH ₃ CH ₂ CH ₂ CH ₃ (n-Butane)	354
CH + cy-C ₆ H ₁₂ (Cyclohexane)	354

CH₂ Reactions:

CH ₂ (X ³ B ₁) + O ₂	354
CH ₂ (a ¹ A ₁) + O ₂	355
CH ₂ (X ³ B ₁) + H ₂	355
CH ₂ (a ¹ B ₁) + H ₂	355
CH ₂ (¹ A ₁) + H ₂ O	355
CH ₂ (X ³ B ₁) + N ₂	355
CH ₂ (X ³ B ₁) + NO	356
CH ₂ (a ¹ A ₁) + NO	356
CH ₂ (X ³ B ₁) + CO	356
CH ₂ (a ¹ A ₁) + CO	356
CH ₂ (X ³ B ₁) + CO ₂	356
CH ₂ (X ³ B ₁) + CH ₃	356
CH ₂ (X ³ B ₁) + CH ₄	357
CH ₂ (X ³ B ₁) + CH ₂ =N=N (Methane, diazo-)	357
CH ₂ (¹ A ₁) + CH ₂ =N=N (Methane, diazo-)	357
CH ₂ (X ³ B ₁) + CH=CH	357
CH ₂ (X ³ B ₁) + CH ₃ CH ₃	358
CH ₂ (a ¹ A ₁) + CH ₂ =C=O (Ketene)	358
CH ₂ (a ¹ B ₁) + CH ₂ =C=O (Ketene)	358
CD ₂ + CD ₂ =C=O (Ketene-d ₂)	359
CH ₂ (X ³ B ₁) + CH ₃ CH ₂ CH ₃	359
CH ₂ (a ¹ A ₁) + CH ₃ CH ₂ CH ₃	360
CH ₂ (a ¹ A ₁) + CH ₂ =CHCH=CH ₂ (1,3-Butadiene)	360
CH ₂ (X ³ B ₁) + CH ₃ CH ₂ CH ₂ CH ₃ (n-Butane)	360
CH ₂ (a ¹ A ₁) + CH ₃ CH ₂ CH ₂ CH ₃ (n-Butane)	361
CH ₂ (X ³ B ₁) + (CH ₃) ₃ CH (Propane, 2-methyl-)	361
CH ₂ (a ¹ A ₁) + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ (n-Pentane)	362
CD ₂ + (CH ₃) ₄ C (Propane, 2,2-dimethyl-)	362

CH₃ RADICAL Reactions:

CH ₃ (+ M)	362
CH ₃ + O ₂ (+ M)	362
CD ₃ + O ₂	365
CH ₃ + O ₃	365
CH ₃ + H ₂	366
CH ₃ [*] + H ₂	366
CH ₃ + HD	366
CH ₃ + D ₂	366
CH ₃ [*] + D ₂	366
CD ₃ + H ₂	366
CD ₃ [*] + H ₂	367
CD ₃ + HD	367
CD ₃ [*] + D ₂	367
CH ₃ + SO ₂ (+ M)	367
CH ₃ + NO (+ M)	367

CH ₃ + NO ₂ (+ M)	368
CH ₃ + N ₂ O	368
CH ₃ + CO (+ M)	368
CH ₃ + CH ₃ (+ M)	369
CH ₃ * + CH ₃	371
CD ₃ + CD ₃ (+ M)	371
CH ₃ + CH ₄	372
CH ₃ + CHO	372
CH ₃ + HCHO (Formaldehyde)	372
CH ₃ + CH ₃ O (Methoxy)	372
CH ₃ + CH ₃ O ₂ (Methyldioxy)	373
CD ₃ + COS	373
CH ₃ + CH ₃ N=NH (Diazene, methyl-)	373
CH ₃ + CH ₃ NO ₂ (Methane, nitro-)	373
CH ₃ + CH≡CH	373
CH ₃ + CH ₂ =CH ₂	373
CH ₃ + CH ₃ CH ₂	374
CH ₃ + CH ₃ CH ₃	374
CH ₃ + CH ₃ CO (Acetyl)	375
CD ₃ + CD ₃ CO (Acetyl-d ₃)	375
CH ₃ + CH ₃ CHO (Acetaldehyde)	376
CH ₃ + CH ₃ CDO (Acetaldehyde-1-d)	376
CH ₃ + HC(O)OCH ₃ (Formic acid methyl ester)	376
CD ₃ + HC(O)OCH ₃ (Formic acid methyl ester)	376
CD ₃ + DC(O)OCH ₃ (Formic-d acid methyl ester)	376
CH ₃ + (CH ₃) ₂ O (Dimethyl ether)	377
CH ₃ + cy-CH ₂ CH ₂ S (Thiirane; Ethylene episulfide)	377
CD ₃ + cy-CH ₂ CH ₂ S (Thiirane; Ethylene episulfide)	377
CH ₃ + (CH ₃) ₂ S (Dimethyl sulfide)	377
CH ₃ + CH ₃ N=NCH ₃ (Azomethane)	378
CD ₃ + CH ₃ N=NCH ₃ (Azomethane)	378
CH ₃ + CH ₂ =C=CH ₂ (Allene)	378
CH ₃ + (CH ₃) ₂ CH (Isopropyl)	378
CH ₃ + CH ₃ CH ₂ CH ₃ (Propane)	378
CH ₃ + CH ₃ C(O)CHO (Propanal, 2-oxo-)	379
CH ₃ + (CH ₃) ₂ CO (2-Propanone)	379
CH ₃ + (CD ₃) ₂ CO (2-Propanone-1,1,1,3,3,3-d ₆)	379
CD ₃ + (CD ₃) ₂ CO (2-Propanone-1,1,1,3,3,3-d ₆)	379
CH ₃ + CH ₃ C(O)OCH ₃ (Methyl acetate)	380
CH ₃ + CH ₃ C(O)OCD ₃ (Methyl-d ₃ acetate)	380
CH ₃ + CD ₃ C(O)OCH ₃ (Methyl acetate-d ₃)	380
CH ₃ + cy-CH(CH ₃)CH ₂ S (Thiirane, methyl-)	380
CH ₃ + (CH ₃) ₂ CHNO ₂ (Propane, 2-nitro-)	381
CH ₃ + CH ₂ C(CH ₃)=CH ₂ (2-Propenyl, 2-methyl-)	381
CH ₃ + trans-CH ₃ CH=CHCH ₃	381
CH ₃ + (CH ₃) ₂ C=CH ₂	381
CH ₃ + (CH ₃) ₃ C (tert-Butyl)	381
CH ₃ + CH ₃ CH ₂ CH ₂ CH ₃ (n-Butane)	381
CH ₃ + (CH ₃) ₃ CH (i-Butane)	382

CH ₃ + CH ₃ C(O)C(O)CH ₃ (Biacetyl)	382
CH ₃ + CD ₃ C(O)C(O)CD ₃ (Biacetyl-d ₆)	383
CD ₃ + CH ₃ C(O)C(O)CH ₃ (Biacetyl)	383
CD ₃ + CD ₂ HC(O)C(O)CD ₃ (Biacetyl-d ₅)	383
CD ₃ + CD ₃ C(O)C(O)CD ₃ (Biacetyl-d ₆)	383
CH ₃ + CH ₃ C(O)CH ₂ CH ₃ (2-Butanone)	384
CH ₃ + CD ₃ C(O)CD ₂ CH ₃ (2-Butanone-1,1,1,3,3-d ₅)	384
CH ₃ + CH ₃ CH ₂ CH ₂ CH=CH ₂ (1-Pentene)	384
CH ₃ + CH ₃ CH ₂ CH=CHCH ₃ (2-Pentene) (Unspecified form)	384
CH ₃ + CH ₃ CH=C(CH ₃) ₂ (2-Butene, 2-methyl-)	385
CH ₃ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ (n-Pentyl)	385
CH ₃ + CH ₃ CH ₂ CH ₂ CHCH ₃ (Butyl, 1-methyl-)	385
CH ₃ + (CH ₃) ₄ C (Neopentane)	385
CH ₃ + CH ₃ C(O)C(O)CH ₂ CH ₃ (2,3-Pentanedione)	386
CH ₃ + CH ₃ CD ₂ C(O)CD ₂ CH ₃ (3-Pentanone-2,2,4,4-d ₄)	386
CH ₃ + CH ₃ CH ₂ CH ₂ C(CH ₃)=CH ₂ (1-Pentene, 2-methyl-)	386
CH ₃ + CH ₃ CH ₂ CH=C(CH ₃) ₂ (2-Pentene, 2-methyl-)	386
CH ₃ + CH ₃ (CH ₂) ₄ CH ₃ (n-Hexane)	387
CH ₃ + (CH ₃) ₂ CHCH(CH ₃) ₂ (Butane, 2,3-dimethyl-)	387
CH ₃ + CH ₃ C(O)CH ₂ CH ₂ C(O)CH ₃ (2,5-Hexanedione)	387
CH ₃ + (CH ₃) ₃ COOC(CH ₃) ₃ (Peroxide, bis(1,1-dimethylethyl)-)	387

CH₄ Reactions:

CH ₄ (+ M)	388
CD ₄ (+ M)	389

CH_xO_y-COMPOUND Reactions:

CHO (+ M)	389
CHO + O ₂ (+ M)	389
CHO + NO	390
CHO + NO ₂	391
CHO + CHO	391
CHO + CH ₃ CH ₂ CH ₂ (n-Propyl)	392
CHO + CH ₃ CH ₂ CH ₂ CHOH (Butyl, 1-hydroxy-)	392
HCHO* (or HC(:)OH) (Formaldehyde (or Methylene, hydroxy-))	392
HCHO (+ M)	392
DCDO (+ M)	393
HCOOH (+ M)	393
HCOOH + HCOOH (Formic acid)	394
CH ₃ O (+ M)	394
CH ₃ O*	394
CH ₃ O + O ₂	394
CH ₃ O + O ₃	395
CH ₃ O + NO	395
CH ₃ O + NO ₂	396
CH ₃ O + N ₂ O	397
CH ₃ O + NH ₃	397

CH ₃ O + CO	397
CH ₃ O + CH ₄	397
CH ₃ O + CH ₃ O	397
CD ₃ O + CD ₃ O	398
CH ₃ O + CH ₃ OH	398
CH ₃ O + CH ₂ =CH ₂	398
CH ₃ O + CH ₃ CO (Acetyl)	398
CH ₃ O + CH ₃ CHO	398
CH ₃ O + CH ₃ OOCH ₃ (Peroxide, dimethyl-)	399
CH ₃ O + (CH ₃) ₃ C (tert-Butyl)	399
CH ₃ O + (CH ₃) ₃ CH	399
CH ₃ O + CH ₃ CH ₂ CH=CH ₂ (1-Butene)	399
CH ₃ O + (CH ₃) ₃ COOH (t-Butyl hydroperoxide)	399
CH ₃ O + (CH ₃) ₂ CHCH(CH ₃) ₂ (Butane, 2,3-dimethyl-)	399
CH ₂ OH (+ M)	399
CH ₂ OH + O ₂	400
CH ₂ OH + H ₂ O	400
CH ₂ OH + H ₂ O ₂	400
CH ₃ O ₂ + O ₃	400
CH ₃ O ₂ + SO ₂	400
CH ₃ O ₂ + NO	401
CH ₃ O ₂ + NO ₂	403
CH ₃ O ₂ + CO	403
CH ₃ O ₂ + HCHO	404
CH ₃ O ₂ + CH ₃ O ₂	404
CD ₃ O ₂ + CD ₃ O ₂	406
CH ₃ O ₂ + CH ₂ =CH ₂	406
CH ₃ O ₂ + CH ₃ C(O)OO (Ethyldioxy, 1-oxo-)	406
CH ₃ O ₂ + CH ₃ N=NCH ₃ (Azomethane)	406
CH ₃ O ₂ + (CH ₃) ₂ CHO ₂ (Ethyldioxy, 1-methyl-)	407
CH ₃ O ₂ + (CH ₃) ₂ C=CH ₂	407
CH ₃ O ₂ + (CH ₃) ₃ CO ₂ (Ethyldioxy, 1,1-dimethyl-)	407
CH ₃ O ₂ + CH ₂ =C(CH ₃)CH ₂ CH ₃ (1-Butene, 2-methyl-)	407
CH ₃ O ₂ + (CH ₃) ₂ C=CHCH ₃ (2-Butene, 2-methyl-)	407
CH ₃ O ₂ + (CH ₃) ₂ C=C(CH ₃) ₂ (2-Butene, 2,3-dimethyl-)	408
CH ₃ O ₂ + (CH ₃) ₂ CHCH(CH ₃) ₂ (Butane, 2,3-dimethyl-)	408
CH ₃ O ₂ + (CH ₃) ₂ CHC(OO·)(CH ₃) ₂ (Propyldioxy, 1,1,3-trimethyl-)	408
HOCH ₂ O + O ₂	408
HOCH ₂ O + NO	408
HOCH ₂ O ₂	409
HOCH ₂ O ₂ + NO	409
HOCH ₂ O ₂ + HOCH ₂ O ₂ (Methyldioxy, hydroxy-)	409
CH ₃ OH (+ M)	409

CS_x-COMPOUND Reactions:

CS ₂ (+ M)	410
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COS Reactions:

COS (+ M)	410
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CH_xS_y-COMPOUND Reactions:

CH ₃ S + CH ₃ S	410
CH ₃ S + cy-CH ₂ CH ₂ S (Thiirane; Ethylene episulfide)	410

CN RADICAL Reactions:

CN (+ M)	411
CN(v=n) + O ₂	411
CN + H ₂	411
CN(v=n) + NO(v'=0)	412
CN(v=n) + NO (+ M)	412
CN + CO ₂	412
CN(v=n) + CH ₄	412
CN + CD ₄	413
CN + COS	413
CN(v=n) + CH≡CH	413
CN + CH ₂ =CH ₂	413
CN + CH ₃ CH ₃	413
CN + NCCN	414
CN + CH ₃ CH=CH ₂	414
CN + CH ₃ CH ₂ CH ₃	414
CN + CH ₂ =CHCH=CH ₂	414

CON-COMPOUND Reactions:

NCO + O ₂	414
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CH_xN_y-COMPOUND Reactions:

HCN (+ M)	414
CH ₃ NH ₂ (+ M)	414
CH ₃ N=N (Diazenyl, methyl-)	415
CH ₃ NHNH ₂ (Hydrazine, methyl-)	415

CH_xO_yN_z-COMPOUND Reactions:

NH ₂ CO (+ M)	415
NH ₂ CO + NH ₂ CO (Amidogen, formyl-)	415
CH ₃ NO† (Methane, nitroso-)	415
CH ₃ ONO (+ M)	415
CH ₃ NO ₂ (+ M)	416
CH ₃ ONO ₂	416

CH ₃ O ₂ NO ₂ (+ M) (Peroxynitric acid methyl ester)	416
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C₂ (Carbon dimer) Reactions:

C ₂ (X ¹ Σ _g ⁺ = A ³ Π _g) (+ M)	417
C ₂ (X ¹ Σ _g ⁺) + O ₂	417
C ₂ (a ³ Π _u) + O ₂	417
C ₂ (X ¹ Σ _g ⁺) + H ₂ O	418
C ₂ (a ³ Π _u) + H ₂ O	418
C ₂ (X ¹ Σ _g ⁺) + N ₂	418
C ₂ (a ³ Π _u) + N ₂	418
C ₂ (X ¹ Σ _g ⁺) + NO	418
C ₂ (a ³ Π _u) + NO	419
C ₂ (X ¹ Σ _g ⁺) + CO ₂	419
C ₂ (a ³ Π _u) + CO ₂	419
C ₂ (X ¹ Σ _g ⁺) + CH ₄	419
C ₂ (a ³ Π _u) + CH ₄	420
C ₂ (X ¹ Σ _g ⁺) + CH=CH	420
C ₂ (a ³ Π _u) + CH=CH	420
C ₂ (X ¹ Σ _g ⁺) + CH ₂ =CH ₂	420
C ₂ (a ³ Π _u) + CH ₂ =CH ₂	421
C ₂ (X ¹ Σ _g ⁺) + CH ₃ CH ₃	421
C ₂ (a ³ Π _u) + CH ₃ CH ₃	421
C ₂ (X ¹ Σ _g ⁺) + CH ₂ =CHCN	421
C ₂ (a ³ Π _u) + CH ₂ =CHCN	421
C ₂ (X ¹ Σ _g ⁺) + CH ₂ =C=CH ₂	421
C ₂ (a ³ Π _u) + CH ₂ =C=CH ₂	422
C ₂ (X ¹ Σ _g ⁺) + CH ₃ CH ₂ CH ₃	422
C ₂ (a ³ Π _u) + CH ₃ CH ₂ CH ₃	422
C ₂ (a ³ Π _u) + CH ₃ CH ₂ CH ₂ CH ₃	422

C₂O Reactions:

C ₂ O + CH=CH	422
C ₂ O + CH ₂ =CH ₂	422
C ₂ O + (CH ₃) ₂ C=CH ₂	423

C₂H_x-COMPOUND Reactions:

CH≡C (+ M)	423
CH≡C + O ₂	423
CH≡C + H ₂	423
CH≡C + CH ₄	424
CH≡C + CH=CH	424
CH≡C + CD≡CD	425
CH≡C + CH ₃ CH ₃	425
CH≡C + CD ₃ CD ₃	425
CH≡C + CH ₃ C≡CH	425
CH≡C + CH≡CC≡CH	425

CH≡C + CH ₂ =CHC≡CH (1-Buten-3-yne)	426
CH≡C + (CH ₃) ₄ C	426
CH≡CH (+ M)	426
CH≡CH + CH≡CH	427
CH≡CH + cy-CH=CHCH=CHCH ₂ (1,3-Cyclopentadiene)	427
CH≡CH + cy-CH ₂ CH ₂ CH=CHCH=CH (1,3-Cyclohexadiene)	427
CH ₂ =CH (+ M)	428
CH ₂ =CH + CH≡CH	428
CH ₂ =CH + CH ₂ =CH	428
CH ₂ =CH + CH ₃ CH ₂	428
CH ₂ =CH ₂ (+ M)	428
CH ₂ =CH ₂ + CH ₂ =CH ₂	429
CH ₂ =CH ₂ + CH ₃ CH=CH ₂	429
CH ₂ =CH ₂ + cis-CH ₃ CH=CHCH ₃	429
CH ₂ =CH ₂ + trans-CH ₃ CH=CHCH ₃	429
CH ₂ =CH ₂ + (CH ₃) ₂ C=CH ₂	430
CH ₂ =CH ₂ + cy-CH=CHCH=CHCH ₂ (1,3-Cyclopentadiene)	430
CH ₂ =CH ₂ + CH ₂ =C(CH ₃)CH=CH ₂ (1,3-Butadiene, 2-methyl-)	430
CH ₂ =CH ₂ + cy-C ₅ H ₈ (Cyclopentene)	430
CH ₂ =CH ₂ + cy-CH ₂ CH ₂ CH=CHCH=CH (1,3-Cyclohexadiene)	431
CH ₃ CH ₂ (+ M)	431
CH ₃ CH ₂ + O ₂	431
CH ₃ CH ₂ + O ₃	432
CH ₃ CH ₂ + H ₂	432
CH ₃ CH ₂ + D ₂	433
CH ₃ CH ₂ + NO	433
CH ₃ CH ₂ + CO	433
CH ₃ CH ₂ + CH ₄	433
CH ₃ CH ₂ + CH ₃ CH ₂	433
CH ₃ CH ₂ + CH ₃ CHO	434
CH ₃ CH ₂ + CH ₃ CH ₂ NO	434
CH ₃ CH ₂ + CH ₃ CH ₂ CHO	434
CH ₃ CH ₂ + CH ₂ =CHCH ₂ CH ₂ (3-Butenyl)	434
CH ₃ CH ₂ + (CH ₃) ₂ C=CH ₂	435
CH ₃ CH ₂ + cy-C ₄ H ₇ (Cyclobutyl)	435
CH ₃ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₃	435
CH ₃ CH ₂ + CH ₃ C(O)C(O)CH ₃ (Biacetyl)	435
CH ₃ CH ₂ + (CH ₃ CH ₂) ₂ O (Diethyl ether)	435
CH ₃ CH ₂ + (CH ₃ CH ₂) ₂ S (Diethyl sulfide)	436
CH ₃ CH ₂ + CH ₃ CH ₂ N=NCH ₂ CH ₃ (Diazene, diethyl-)	436
CH ₃ CH ₂ + (CH ₃ CH ₂) ₂ NOH (Ethanamine, N-ethyl-N-hydroxy-)	436
CH ₃ CH ₂ + cy-CH ₂ CH ₂ CH=CHCH (2-Cyclopenten-1-yl)	436
CH ₃ CH ₂ + CH ₃ CH=CHCH ₂ CH ₂ (3-Pentenyl)	437
CH ₃ CH ₂ + cy-C ₅ H ₉ (Cyclopentyl)	437
CH ₃ CH ₂ + CH ₃ C(O)C(O)CH ₂ CH ₃ (2,3-Pentanedione)	437
CH ₃ CH ₂ + cy-C ₆ H ₁₁ (Cyclohexyl)	438
CH ₃ CH ₂ + n-C ₆ H ₁₄ (n-Hexane)	438
CH ₃ CH ₃ (+ M)	438
CH ₃ CH ₃ †	440

CD ₃ CD ₃	440
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C₂H_xO_y-COMPOUND Reactions:

CH=C=O + O ₂	440
CH=C=O + CH≡CH	440
CH ₂ =C=O + CH ₂ =C=O	441
CH ₂ =C=O + CH ₃ COOH	441
CH ₂ =C=O + CH ₃ CH ₂ COOH	441
CH ₂ =C=O + CH ₃ CH ₂ CH ₂ COOH (Butanoic acid)	441
CH ₂ =C=O + (CH ₃) ₂ CHCOOH (Propanoic acid, 2-methyl-)	441
CH ₂ =C=O + (CH ₃) ₃ CCOOH (Propanoic acid, 2,2-dimethyl-)	441
CH ₂ =C=O + (CH ₃) ₃ CCH ₂ COOH (Butanoic acid, 3,3-dimethyl-)	441
CH ₃ CO (+ M)	441
CH ₃ CO + O ₂	442
CH ₃ CO + NO	442
CH ₃ CO + NO ₂	442
CH ₃ CO + CH ₃ CO	442
CD ₃ CO + CD ₃ CO	443
CH ₃ CO + CH ₃ CHO	443
CH ₃ CO + CH ₂ =CHCH=CH ₂	443
CH ₃ C(O)O + NO ₂	444
CH ₃ C(O)OO + NO	444
CH ₃ C(O)OO + NO ₂	444
CH ₃ C(O)OO + HCHO	444
CH ₃ C(O)OO + CH ₃ C(O)OO	445
CH ₃ C(O)OO + CH ₃ CH=CH ₂	445
CH ₃ C(O)OO + CH ₃ CH ₂ CH=CH ₂	445
CH ₃ C(O)OO + cis-CH ₃ CH=CHCH ₃	445
CH ₃ C(O)OO + trans-CH ₃ CH=CHCH ₃	445
CH ₃ C(O)OO + (CH ₃) ₂ C=CH ₂	445
CH ₃ C(O)OO + cis-CH ₃ CH=CHCH ₂ CH ₃	446
CH ₃ C(O)OO + trans-CH ₃ CH=CHCH ₂ CH ₃	446
CH ₃ C(O)OO + CH ₃ CH ₂ C(CH ₃)=CH ₂ (1-Butene, 2-methyl-)	446
CH ₃ C(O)OO + (CH ₃) ₂ CHCH=CH ₂ (1-Butene, 3-methyl-)	446
CH ₃ C(O)OO + (CH ₃) ₂ C=CHCH ₃ (2-Butene, 2-methyl-)	446
CH ₃ C(O)OO + CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Hexene)	446
CH ₃ CHO (+ M)	447
CH ₃ CHO + CH ₃ C(O)OOH (Ethaneperoxoic acid)	447
CH ₃ C(O)OOH + CH ₃ CH=CH ₂	447
CH ₃ C(O)OOH + CH ₃ CH ₂ CH=CH ₂	447
CH ₃ C(O)OOH + cis-CH ₃ CH=CHCH ₃	447
CH ₃ C(O)OOH + trans-CH ₃ CH=CHCH ₃	448
CH ₃ C(O)OOH + (CH ₃) ₂ C=CHCH ₃	448
CH ₃ C(O)OOH + cis-CH ₃ CH=CHCH ₂ CH ₃	448
CH ₃ C(O)OOH + trans-CH ₃ CH=CHCH ₂ CH ₃	448
CH ₃ C(O)OOH + CH ₃ CH ₂ C(CH ₃)=CH ₂ (1-Butene, 2-methyl-)	448
CH ₃ C(O)OOH + (CH ₃) ₂ CHCH=CH ₂ (1-Butene, 3-methyl-)	449
CH ₃ C(O)OOH + (CH ₃) ₂ C=CHCH ₃ (2-Butene, 2-methyl-)	449

CH ₃ C(O)OOH + CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Hexene)	449
CH ₃ CH ₂ O (Ethoxy)	449
CH ₃ CH ₂ O + O ₂	450
CH ₃ CH ₂ O + NO	450
CH ₃ CH ₂ O + NO ₂	450
CH ₃ CHOH (+ M)	450
CH ₃ CHOH (Ethyl, 1-hydroxy-) + O ₂	450
CH ₃ CH ₂ O ₂ (Ethyldioxy)	451
CH ₃ CH ₂ O ₂ + NO	451
CH ₃ CH ₂ O ₂ + NO ₂	451
CH ₃ CH ₂ O ₂ + CH ₂ =CH ₂	452
CH ₃ CH ₂ O ₂ + CH ₃ CH ₂ O ₂	452
CH ₃ CH ₂ OH (+ M)	452
(CH ₃) ₂ O	452
CH ₃ OOCH ₃ (Peroxide, dimethyl-)	453

C₂H_xS_y-COMPOUND Reactions:

cy-CH ₂ CH ₂ S (Thiirane; Ethylene episulfide)	453
cy-CH ₂ CH ₂ S* (Thiirane; Ethylene episulfide)	453
CH ₃ SCH ₂ + CH ₄	454

C₂N_x-COMPOUND Reactions:

NCCN (+ M)	454
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C₂H_xN_y-COMPOUND Reactions:

CH ₃ NC (Methane, isocyano-)	454
(CH ₃) ₂ N + O ₂	454
(CH ₃) ₂ N + NO ₂	454
CH ₃ N=NCH ₃ (Azomethane; Diazene, dimethyl-)	454
CH ₃ N=NCH ₃ * (Azomethane; Diazene, dimethyl-)	455
(CH ₃) ₂ NNH ₂ (Hydrazine, 1,1-dimethyl-)	455
CH ₃ NHNHCH ₃ (Hydrazine, 1,2-dimethyl-)	455

C₂H_xO_yN_z-COMPOUND Reactions:

CH ₃ C(O)OONO ₂ (Peroxide, acetyl nitro-)	455
CH ₃ CH ₂ NO + CH ₃ CH ₂ NO (Ethane, nitroso-)	455
CH ₃ CH ₂ NO ₂ (Ethane, nitro-) (+ M)	455
CH ₃ CH ₂ ONO	456
CH ₃ CH ₂ ONO ₂	456

C₃ (Carbon trimer) Reactions:

C ₃ + O ₂	456
C ₃ + N ₂	456
C ₃ + NO	457

$C_3 + CH_4$	457
$C_3 + CH=CH$	457
$C_3 + CH_2=CH_2$	457
$C_3 + CH_3CH_3$	458
$C_3 + CH_3C\equiv CH$	458
$C_3 + CH_2=C=CH_2$	458
$C_3 + CH_3CH=CH_2$	458
$C_3 + CH_3CH_2CH=CH_2$	459
$C_3 + cis-CH_3CH=CHCH_3$	459
$C_3 + (CH_3)_2C=CH_2$	459
$C_3 + CH_3CH_2CH_2CH_3$	460
$C_3 + CH_3CH_2CH_2C\equiv CH$	460
$C_3 + CH_3CH=C=CHCH_3$ (2,3-Pentadiene)	460
$C_3 + (CH_3)_2C=CHCH_3$	460
$C_3 + CH_3CH_2CH_2C\equiv CCH_3$ (2-Hexyne)	460
$C_3 + (CH_3)_2C=C(CH_3)_2$	461
$C_3 + (CH_3)_2C=C=C(CH_3)_2$ (2,3-Pentadiene, 2,4-dimethyl-)	461

C_3H_x -COMPOUND Reactions:

$CH_3C\equiv CD$	461
$CH_2DC\equiv CH$	461
$CH_2=C=CH_2$ (+ M)	462
$CH_2=C=CHD$	462
cy- C_3H_4 (Cyclopropene)	462
$CH_3CH=CH^\dagger$ (1-Propenyl)	462
$CH_2=CHCH_2^\dagger$ (Allyl)	463
$CD_2=CDCD_2^\dagger$	463
$CH_2=CHCH_2 + O_2$	463
$CH_2=CHCH_2 + NO$ (+ M)	463
$CH_2=CHCH_2 + NO_2$	464
$CH_2=CHCH_2 + CH\equiv CH$	464
$CH_2=CHCH_2 + CH_2=CH_2$	464
$CH_2=CHCH_2 + CH\equiv CCH_3$	465
$CH_2=CHCH_2 + CH_2=CHCH_2$	466
$CH_3CH=CH_2$ (+ M)	466
$CH_3CH=CH_2^\dagger$	467
$CH_3CH=CH_2 + CH_3CH=CH_2$	467
$CH_3CH=CH_2 + cy-CH_2CH_2CH=CHCH=CH$ (1,3-Cyclohexadiene)	467
cy- C_3H_6 (Cyclopropane)	468
(+)-trans-cy- $CH_2CHDCHD$ (Cyclopropane-1,2- d_2 , (1S-trans)-)	469
(-)-trans-cy- $CH_2CHDCHD$ (Cyclopropane-1,2- d_2 , (1R-trans)-)	469
$CH_3CH_2CH_2$ (n-Propyl) (+ M)	470
$CH_3CH_2CH_2 + O_2$	470
$CH_3CH_2CH_2 + O_3$	471
$CH_3CH_2CH_2 + HCHO$	471
$CH_3CH_2CH_2 + CH\equiv CH$	471
$CH_3CH_2CH_2 + CH_2=CH_2$	471
$CH_3CH_2CH_2 + CH_3CH_2CH_2$	471

$\text{CH}_3\text{CH}_2\text{CH}_2 + (\text{CH}_3)_2\text{CH}$	472
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO}$	472
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (n-Pentyl)	472
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3$ (Butyl, 1-methyl-)	472
$(\text{CH}_3)_2\text{CH}$ (i-Propyl)	473
$(\text{CH}_3)_2\text{CH}^\dagger$	473
$(\text{CH}_3)_2\text{CH} + \text{O}_2$	473
$(\text{CH}_3)_2\text{CH} + \text{O}_3$	473
$(\text{CH}_3)_2\text{CH} + \text{H}_2$	474
$(\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}_3$	474
$(\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}=\text{CH}_2$	474
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH}$	474
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CHCHO}$ (Propanal, 2-methyl-)	475
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_4\text{C}$	475
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ (Butane, 2,3-dimethyl-)	475
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2$ (Azoisopropane)	476
$\text{CH}_3\text{CH}_2\text{CH}_3 (+ \text{M})$	476
$\text{CH}_3\text{CH}_2\text{CH}_3^\dagger$	477
$\text{CD}_3\text{CD}_2\text{CD}_3$	477

$\text{C}_3\text{H}_x\text{O}_y$ -COMPOUND Reactions:

$\text{CH}_2=\text{CHCHO} + \text{cy-CH}_2\text{CH}_2\text{CH}=\text{CHCH}=\text{CH}$ (1,3-Cyclohexadiene)	477
$\text{CH}_3\text{CH}_2\text{CO} (+ \text{M})$	478
$\text{CH}_3\text{CH}_2\text{CO} + \text{O}_2$	478
$\text{CH}_2=\text{CHCH}_2\text{O}_2$ (2-Propenyldioxy)	478
$\text{CH}_3\text{CH}_2\text{CHO} + \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OOH}$ (Propaneperoxoic acid)	478
$\text{cy-CH}_2\text{CH}_2\text{CH}_2\text{O}$ (Oxetane)	478
$\text{cy-CH}(\text{CH}_3)\text{CH}_2\text{O}$ (Oxirane, methyl-)	479
$\text{HC}(\text{O})\text{OCH}_2\text{CH}_3$ (Ethyl formate)	479
$\text{CH}_3\text{C}(\text{O}^{18})\text{OCH}_3$ (Acetic- ^{18}O acid ^{16}O -methyl ester)	479
$\text{CH}_3\text{C}(\text{O})\text{OCH}_3$ (Methyl acetate)	479
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO}$	480
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO}_2$	480
$(\text{CH}_3)_2\text{CHO}$ (Ethoxy, 1-methyl-)	480
$(\text{CH}_3)_2\text{CHO} + \text{NO}$	480
$(\text{CH}_3)_2\text{CHO} + (\text{CH}_3)_2\text{CHOOH}$ (Ethoxy, 1-methyl- + Hydroperoxide, 1-methylethyl-)	481
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{O}_2$	481
$(\text{CH}_3)_2\text{CHO}_2$ (Ethyldioxy, 1-methyl-) + NO	481
$(\text{CH}_3)_2\text{CHO}_2 + \text{NO}_2$	481
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHO}_2$	482
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$	482
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ (Ethyldioxy, 1-methyl- + Propyldioxy, 1,1,2-trimethyl-)	483
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$ (1-Propanol)	483
$(\text{CH}_3)_2\text{CHOH}$ (2-Propanol)	483

C₃H_xS_y-COMPOUND Reactions:

cy-CH₂CH₂CH₂S (Thietane; Trimethylene sulfide) 483

C₃H_xO_yS_z-COMPOUND Reactions:

CH₃C(S)OCH₃ (Ethanethioic acid O-methyl ester) 484

cy-CH₂CH₂CH₂S(O₂) (Thietane, 1,1-dioxide-;
Trimethylenesulfone) 484

C₃H_xN_y-COMPOUND Reactions:

CH₂=CHCN + NH₂CH₂CH₂CN (Acrylonitrile; 2-Propenenitrile) +
(β-Aminopropionitrile; Propanenitrile, 3-amino-) 484

CH₃CH₂CN (Propanenitrile) 484

cy-CH₂CH₂CH(NH₂) (Cyclopropanamine) 485

C₃H_xO_yN_z-COMPOUND Reactions:

(CH₃)₂CHONO (Nitrous acid 1-methylethyl ester;
Isopropyl nitrite) 485

CH₃NHC(O)OCH₃ (Carbamic acid, methyl-, methyl ester) 486

CH₃CH₂CH₂ONO₂ (Nitric acid propyl ester; n-Propyl nitrate) . 486

C₄H_x-COMPOUND Reactions:

CH=CC=C 486

CH=CC=C + CH=CC=CH 486

CH=CC=CH 486

CH₃CH₂C=CH 487

CH₃CH₂C=CH + CH₃CH₂C=CH 487

CH₂=CHCH=CH₂ + CH₂=CHCH=CH₂ 487

CH₂=CHCH=CH₂ + cy-CH₂CH₂CH=CHCH=CH (1,3-Cyclohexadiene) 488

CH₃CH₂CH=CH[†] (1-Butenyl) 488

CH₃CH=CHCH₂ + H₂S 489

CH₃CH=CHCH₂ + cis-CH₃CH=CHCH₃ 489

trans-CH₃CH=CHCH₂ 489

CH₂=CHCH₂CH₂[†] (3-Butenyl) 489

CH₂=CHCH₂CH₂ + cy-C₄H₇ (Cyclobutyl) 489

CH₃C=CHCH₃[†] (1-Propenyl, 1-methyl-) 490

CH₂=CHCHCH₃[†] (2-Propenyl, 1-methyl-) 490

trans-CH₃CHCH=CH₂ (2-Propenyl, 1-methyl-, (E)-) 490

CH₂=CHCHCH₃ + CH₂=CHCHCH₃ (1-Methylallyl) 490

CH₂C(CH₃)=CH₂ (2-Methylallyl) 490

CH₂=C(CH₃)CH₂ + CH₂=C(CH₃)CH₂ (2-Methylallyl) 491

cy-C₄H₇ + cy-C₄H₇ (Cyclobutyl + Cyclobutyl) 491

CH₃CH₂CH=CH₂ 491

cis-CH₃CH=CHCH₃ (+ M) 491

cis-CH ₃ CH=CHCH ₃ + H ₂ S	492
trans-CH ₃ CH=CHCH ₃ (+ M)	492
(CH ₃) ₂ C=CH ₂	492
CH ₂ CH ₂ CH ₂ CH ₂ (1,4-Butanediyl)	493
cy-C ₄ H ₈ (Cyclobutane)	493
CH ₃ CH ₂ CH ₂ CH ₂ (n-Butyl)	494
CH ₃ CH ₂ CH ₂ CH ₂ + O ₂	494
CH ₃ CH ₂ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₂ (n-Butyl)	494
CH ₃ CH ₂ CH ₂ CH ₂ + CH ₃ CH ₂ CHCH ₃ (n-Butyl + Propyl, 1-methyl-)	495
CH ₃ CH ₂ CHCH ₃ (Propyl, 1-methyl-)	495
CH ₃ CH ₂ CHCH ₃ + O ₂	495
CH ₃ CH ₂ CHCH ₃ + CH ₃ CH ₂ CHCH ₃ (Propyl, 1-methyl- + Propyl, 1-methyl-)	496
(CH ₃) ₂ CHCH ₂ (Propyl, 2-methyl-) + O ₂	496
(CH ₃) ₃ C (t-Butyl)	496
(CH ₃) ₃ C + O ₂	497
(CH ₃) ₃ C + O ₃	497
(CH ₃) ₃ C + H ₂	498
(CH ₃) ₃ C + NO	498
(CH ₃) ₃ C + (CH ₃) ₃ C	498
CH ₃ CH ₂ CH ₂ CH ₃	499
(CH ₃) ₃ CH (Isobutane)	499
(CH ₃) ₃ CH [†] (Isobutane)	500

C₄H_xO_y-COMPOUND Reactions:

CH=CCH ₂ COOH (3-Butynoic acid)	500
CH=CCH ₂ COOD (3-Butynoic acid-d)	500
CH ₂ C(O)C(O)CH ₃ (Butyl, 2,3-dioxo-)	501
cy-CH ₂ CH ₂ CH ₂ C(O) (Cyclobutanone)	501
(+)-(S)-cy-CH(CH=CH ₂)CH ₂ O (Oxirane, ethenyl-, (S)-)	501
(S)-cis-cy-CH(CH=CH ₂)CHDO (Oxirane-d, 3-ethenyl-, cis-, (S)-)	502
trans-cy-CH(CH=CH ₂)CHDO (Oxirane-d, 3-ethenyl-, trans-)	502
cy-CH(CH=CH ₂)CD ₂ O (Oxirane-2,2-d ₂ , ethenyl-)	503
CH ₂ =CHCH ₂ COOH (3-Butenoic acid)	503
CH ₃ C(O)C(O)CH ₃ (2,3-Butanedione)	503
CH ₃ CH ₂ CH ₂ CO (Butyl, 1-oxo-)	503
CH ₂ CH ₂ C(O)CH ₃ (Butyl, 3-oxo-)	503
CH ₃ CH ₂ CHCHO (Propyl, 1-formyl-)	504
(CH ₃) ₂ CCHO (Ethyl, 1,1-dimethyl-2-oxo-) (+ M)	504
CH ₃ CH(OH)CH=CH ₂ (3-Buten-2-ol)	504
CH ₃ OCH ₂ CH=CH ₂ (1-Propene, 3-methoxy-)	504
CH ₃ CH ₂ OCH=CH ₂ (Ethene, ethoxy-)	504
CH ₃ CH ₂ C(O)CH ₃ (+ M)	504
cy-CH(CH ₂ CH ₃)CH ₂ O (Oxirane, ethyl-)	505
cy-C(CH ₃) ₂ CH ₂ O (Oxirane, 2,2-dimethyl-)	505
cis-cy-CH(CH ₃)CH(CH ₃)O (Oxirane, 2,3-dimethyl-, cis-; cis-2,3-Epoxybutane)	506

trans-cy-CH(CH ₃)CH(CH ₃)O (Oxirane, 2,3-dimethyl-, trans-; trans-2,3-Epoxybutane)	506
cy-CH ₂ CH ₂ CH(CH ₃)O (Oxetane, 2-methyl-)	507
CH ₃ C(O)OCH ₂ CH ₃ (Ethyl acetate)	507
CH ₃ OC(O)OCH ₂ CH ₃ (Carbonic acid ethyl methyl ester)	508
CH ₃ CH(OH)CHCH ₃ (Propyl, 2-hydroxy-1-methyl-) + O ₂	508
CH ₃ CH ₂ CH ₂ CH ₂ O (Butoxy)	508
CH ₃ CH ₂ CH(O·)CH ₃ (Propoxy, 1-methyl-)	508
CH ₃ CH ₂ CH(O·)CH ₃ + NO	508
CH ₃ CH ₂ CH(O·)CH ₃ + NO ₂	509
(CH ₃) ₃ CO (t-Butoxy)	509
(CH ₃) ₃ CO + NO	509
(CH ₃) ₃ CO + HCHO	510
(CH ₃) ₃ CO + CH ₃ CHO	510
(CH ₃) ₃ CO + CD ₃ CHO	510
(CH ₃) ₃ CO + (CH ₃) ₂ CO	511
(CH ₃) ₃ CO + (CD ₃) ₂ CO	511
(CH ₃) ₃ CO + (CH ₃) ₃ CH	511
(CH ₃) ₃ CO ₂ + NO	511
(CH ₃) ₃ CO ₂ + NO ₂	512
(CH ₃) ₃ CO ₂ + (CH ₃) ₃ CO ₂	512
(CH ₃) ₂ CCH ₂ OOH (Ethyl, 1-(hydroperoxymethyl)-1-methyl-)	512
(CH ₃) ₂ CHCH ₂ O ₂ (Propyldioxy, 2-methyl-)	513
(CH ₃) ₂ C(OO·)CH ₂ OOH (Ethyldioxy, 1-(hydroperoxymethyl)-1-methyl)	513
(CH ₃) ₃ COH (t-Butanol)	513
(CH ₃ CH ₂) ₂ O (Diethyl ether)	513

C₄H_xS_y-COMPOUND Reactions:

CH ₃ SCH ₂ CH=CH ₂ (1-Propene, 3-(methylthio)-)	514
CH ₃ C(S)SCH ₂ CH ₃ (Ethane(dithioic) acid ethyl ester)	514

C₄H_xO_yS_z-COMPOUND Reactions:

CH ₃ C(O)SCH ₂ CH ₃ (Ethanethioic acid S-ethyl ester)	514
CH ₃ C(S)OCH ₂ CH ₃ (Ethanethioic acid O-ethyl ester)	514
CH ₃ OC(S)OCH ₂ CH ₃ (Carbonothioic acid O-ethyl O-methyl ester)	515
CH ₃ OC(O)SCH ₂ CH ₃ (Carbonothioic acid S-ethyl O-methyl ester)	515
CH ₃ CH ₂ OC(O)SCH ₃ (Carbonothioic acid O-ethyl S-methyl ester)	515
CH ₃ SC(S)OCH ₂ CH ₃ (Carbonodithioic acid O-ethyl S-methyl ester)	515

C₄H_xN_y-COMPOUND Reactions:

CH ₂ =CHCH ₂ NC (1-Propene, 3-isocyano-)	515
cis-CH ₃ CH=CHCN (cis-Crotononitrile)	516
cy-CH ₂ CH ₂ CH(CN) (Cyclopropanecarbonitrile; Cyclopropyl cyanide)	516
CH ₃ CH ₂ CH ₂ CN (Butanenitrile)	516

$(\text{CH}_3)_2\text{CHCN}$ (Propanenitrile, 2-methyl-)	516
$\text{CH}_2=\text{CHCH}_2\text{NHCH}_3$ (2-Propen-1-amine, N-methyl-)	517
$\text{CH}_3\text{N}=\text{NCH}_2\text{CH}=\text{CH}_2$ (Diazene, methyl-(2-propenyl)-)	517
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3$ (Azoethane)	517
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3^*$ (Azoethane)	517
$(\text{CH}_3)_2\text{NN}(\text{CH}_3)_2$ (Hydrazine, tetramethyl-)	517

$\text{C}_4\text{H}_x\text{O}_y\text{N}_z$ -COMPOUND Reactions:

$\text{NCC}(\text{O})\text{OCH}_2\text{CH}_3$ (Ethyl cyanofornate)	518
$(\text{CH}_3)_3\text{CNO}$	518
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO}$ (n-Butyl nitrite)	518
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{ONO}$ (s-Butyl nitrite)	518
$(\text{CH}_3)_3\text{CONO}$ (t-Butyl nitrite)	518
$(\text{CH}_3)_3\text{CONO}_2$ (t-Butyl nitrate)	519
$(\text{CH}_3\text{CH}_2)_2\text{NO}$ (Nitroxide, diethyl-) + NO_2	519
$(\text{CH}_3\text{CH}_2)_2\text{NOH}$ (Ethanamine, N-ethyl-N-hydroxy-) + NO_2	519
$(\text{CH}_3\text{CH}_2\text{NO})_2$ (Nitrosoethane dimer; Diazene, diethyl-, 1,2-dioxide)	519

C_5H_x -COMPOUND Reactions:

$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH}$ (1-Pentyne)	520
$\text{CH}_3\text{CH}_2\text{C}\equiv\text{CCH}_3$ (2-Pentyne)	520
$(\text{CH}_3)_2\text{CHC}\equiv\text{CH}$ (1-Butyne, 3-methyl-)	520
cis- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (cis-1,3-Pentadiene)	520
cis- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2^\dagger$ (cis-1,3-Pentadiene)	521
trans- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (trans-1,3-Pentadiene)	521
$(\text{CH}_3)_2\text{C}=\text{C}=\text{CH}_2$ (1,2-Butadiene, 3-methyl-)	521
cy- C_5H_8 (Cyclopentene)	521
cy- $\text{CH}(\text{CH}=\text{CH}_2)\text{CH}_2\text{CH}_2\text{O}$ (Cyclopropane, ethenyl-)	522
$(\text{CH}_2)_2>\text{C}<(\text{CH}_2)_2$ (Spiropentane)	522
$[\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3 = \text{CH}_2=\text{CHCHCH}_2\text{CH}_3]$ (2-Pentenyl = 2-Propenyl, 1-ethyl-)	523
$[\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3 = \text{CH}_2=\text{CHCHCH}_2\text{CH}_3]$ (2-Pentenyl = 2-Propenyl, 1-ethyl-) + O_2	523
$\text{CH}_2\text{CH}=\text{CHCH}_2\text{CH}_3$ (2-Pentenyl) + CH_3CHO	523
$\text{CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2$ (3-Pentenyl)	523
$\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger$ (4-Pentenyl)	524
$\text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2^\dagger$ (3-Butenyl, 1-methyl-)	524
$\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2^\dagger$ (3-Butenyl, 2-methyl-)	524
cy- C_5H_9 + cy- C_5H_9 (Cyclopentyl + Cyclopentyl)	524
cy- C_5D_9 + cy- C_5D_9 (Cyclopentyl-d ₉ + Cyclopentyl-d ₉)	525
cy- C_5H_9 + cy- C_6H_{11} (Cyclopentyl + Cyclohexyl)	525
cy- C_5H_9 + cy- C_6D_{11} (Cyclopentyl + Cyclohexyl-d ₁₁)	526
cy- C_5D_9 + cy- C_6H_{11} (Cyclopentyl-d ₉ + Cyclohexyl)	526
cy- C_5D_9 + cy- C_6D_{11} (Cyclopentyl-d ₉ + Cyclohexyl-d ₁₁)	527
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (1-Pentene)	527
$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$ (2-Pentene, cis-trans mixture)	528

cis-CH ₃ CH ₂ CH=CHCH ₃ (cis-2-Pentene) (+ M)	528
trans-CH ₃ CH ₂ CH=CHCH ₃ (trans-2-Pentene) (+ M)	528
CH ₃ CH ₂ C(CH ₃)=CH ₂ (1-Butene, 2-methyl-)	528
CH ₃ CH ₂ C(CH ₃)=CH ₂ [†] (1-Butene, 2-methyl-)	528
(CH ₃) ₂ CHCH=CH ₂ [†] (1-Butene, 3-methyl-)	529
cy-C ₅ H ₁₀ (Cyclopentane)	529
cis-cy-CH(CH ₃)CH(CH ₃)CH ₂ (Cyclopropane, 1,2-dimethyl-, cis-)	530
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (Pentyl)	530
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ [†] (Pentyl)	530
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (Pentyl) + O ₂	530
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (Pentyl + Pentyl)	531
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ N=NCH ₃ (Diazene, methylpentyl-)	531
CH ₃ CH ₂ CH ₂ CHCH ₃ (Butyl, 1-methyl-)	531
CH ₃ CH ₂ CH ₂ CHCH ₃ [†] (Butyl, 1-methyl-)	531
CD ₃ CD ₂ CD ₂ CD ₂ CD ₃ [†] (Butyl-1,2,2,3,3,4,4,4-d ₈ , 1-methyl-d ₃)	531
CH ₃ CH ₂ CH ₂ CHCH ₃ (Butyl, 1-methyl-) + O ₂	532
CH ₃ CH ₂ CH ₂ CHCH ₃ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (Butyl, 1-methyl- + Pentyl)	532
CH ₃ CH ₂ CHCH ₂ CH ₃ (Propyl, 1-ethyl-)	532
CH ₃ CH ₂ CHCH ₂ CH ₃ (Propyl, 1-ethyl-) + O ₂	532
(CH ₃) ₃ CCH ₂ (Propyl, 2,2-dimethyl-) (+ M)	532
CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ (n-Pentane)	533
CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ [†] (n-Pentane)	533
(CH ₃) ₂ CHCH ₂ CH ₃ [†] (Isopentane)	533
(CH ₃) ₄ C (Neopentane)	534

C₅H_xO_y-COMPOUND Reactions:

CH ₃ C≡CCH ₂ COOH (3-Pentynoic acid)	534
CH ₃ C≡CCH ₂ COOD (3-Pentynoic acid-d)	534
CH ₂ =C=CHCH ₂ COOH (3,4-Pentadienoic acid)	534
cy-CH ₂ CH ₂ CH=C(CH ₃)O (Furan, 2,3-dihydro-5-methyl-)	535
(cy-CH ₂ CH ₂ CH)C(O)CH ₃ (Ethanone, 1-cyclopropyl-)	535
bicy-C ₅ H ₈ O (6-Oxabicyclo[3.1.0]hexane)	535
CH ₃ CH=CHCH ₂ COOH (3-Pentenoic acid)	536
CH ₃ C(O)C(O)CH ₂ CH ₃ (2,3-Pentanedione)	536
CH ₂ =C(CH ₃)CH ₂ COOH (3-Butenoic acid, 3-methyl-)	536
(cy-CH ₂ CH ₂ CH)CH ₂ COOH (Cyclopropaneacetic acid)	536
CH ₃ CH ₂ OCH ₂ CH=CH ₂ (1-Propene, 3-ethoxy-)	537
CH ₃ CH ₂ CH ₂ OCH=CH ₂ (Propane, 1-(ethenyloxy)-)	537
cy-CH ₂ CH ₂ CH(CH ₂ CH ₃)O (Oxetane, 2-ethyl-)	537
cy-CH ₂ CH ₂ C(CH ₃) ₂ O (Oxetane, 2,2-dimethyl-)	537
cis-cy-CH ₂ CH(CH ₃)CH(CH ₃)O (Oxetane, 2,3-dimethyl-, cis-)	538
trans-cy-CH ₂ CH(CH ₃)CH(CH ₃)O (Oxetane, 2,3-dimethyl-, trans-)	538
cy-CH(CH ₃)C(CH ₃) ₂ O (Oxirane, trimethyl-)	538
CH ₃ OCH ₂ CH ₂ OCH=CH ₂ (Ethene, (2-methoxyethoxy)-)	539
CH ₃ C(O)OCH ₂ CH ₂ CH ₃ (n-Propyl acetate)	539
CH ₃ C(O)OCH(CH ₃) ₂ (i-Propyl acetate)	539
CH ₃ CH ₂ C(O)OCH ₂ CH ₃ (Propanoic acid ethyl ester)	539

$\text{CH}_3\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_3$	(Carbonic acid diethyl ester)	540
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{OCH}_3$	(Ethanol, 2-(methoxy)-, acetate)	540
$\text{HOCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Acetic acid, hydroxy-, 1-methylethyl ester)	540
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{O}$	(Propoxy, 1,1-dimethyl-)	540
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{O} + \text{NO}$	(Propoxy, 1,1-dimethyl-)	540
$(\text{CH}_3)_3\text{CCH}_2\text{OO}$	(Propyldioxy, 2,2-dimethyl-)	541
$\text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{CHCH}_3$	(Butyl, 3-hydroperoxy-1-methyl-)	541
$\text{HOOCH}_2\text{CH}_2\text{CHCH}_2\text{CH}_3$	(Propyl, 3-hydroperoxy-1-ethyl-)	541
$(\text{CH}_3)_2\text{C}(\text{CH}_2\text{OOH})\text{CH}_2$	(Propyl, 2-methyl-2-hydroperoxymethyl-)	541
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO}$	(Pentyldioxy)	541
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{O}_2)\text{CH}_3$	(Butyldioxy, 1-methyl-)	542
$\text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{CH}(\text{OO}\cdot)\text{CH}_3$	(Butyldioxy, 3-hydroperoxy-1-methyl-)	542
$\text{CH}_3\text{CH}_2\text{CH}(\text{OO})\text{CH}_2\text{CH}_2\text{OOH}$	(Propyldioxy, 3-hydroperoxy-1-ethyl-)	542
$(\text{CH}_3)_2\text{C}(\text{CH}_2\text{OOH})\text{CH}_2\text{OO}$	(Propyldioxy, 2-hydroperoxymethyl-2-methyl-)	542
$(\text{CH}_3)_3\text{COCH}_3$	(Propane, 2-methoxy-2-methyl-)	542

$\text{C}_5\text{H}_x\text{O}_y\text{S}_z$ -COMPOUND Reactions:

$\text{CH}_3\text{C}(\text{O})\text{SCH}(\text{CH}_3)_2$	(Ethanethioic acid S-(1-methylethyl) ester)	543
$\text{CH}_3\text{C}(\text{S})\text{OCH}(\text{CH}_3)_2$	(Ethanethioic acid O-(1-methylethyl) ester)	543
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{SCH}_3$	(Ethanol, 2-(methylthio)-, acetate)	543
$\text{CH}_3\text{C}(\text{O})\text{SCH}(\text{CH}_3)\text{OCH}_3$	(Ethanethioic acid S-(1-methoxyethyl ester)	543
$\text{CH}_3\text{OC}(\text{S})\text{OCH}(\text{CH}_3)_2$	(Carbonothioic acid O-methyl O-(1-methylethyl) ester)	543
$\text{CH}_3\text{OC}(\text{O})\text{SCH}(\text{CH}_3)_2$	(Carbonothioic acid O-methyl S-(1-methylethyl) ester)	544
$(\text{CH}_3)_2\text{CHOC}(\text{O})\text{SCH}_3$	(Carbonothioic acid S-methyl O-(1-methylethyl) ester)	544
cy- $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{S}(\text{O}_2)$	(Thiophene, tetrahydro-3-methyl- 1,1-dioxide; 3-Methylsulfolane)	544
$\text{CH}_3\text{SC}(\text{S})\text{OCH}(\text{CH}_3)_2$	(Carbonodithioic acid S-methyl O-(1-methylethyl) ester)	544
$\text{CH}_3\text{OC}(\text{S})\text{SCH}(\text{CH}_3)_2$	(Carbonodithioic acid O-methyl S-(1-methylethyl) ester)	544

$\text{C}_5\text{H}_x\text{N}_y$ -COMPOUND Reactions:

cy- $\text{CH}_2\text{CH}_2\text{CH}=\text{CHC}(\text{CN})$	(1-Cyclobutene-1-carbonitrile)	545
bicy- $\text{C}_4\text{H}_5(\text{CN})$	(Bicyclo[1.1.0]butane-1-carbonitrile)	545
cy- $\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\text{CN})$	(Cyclobutanecarbonitrile)	545
$(\text{CH}_3)_2\text{CHCH}_2\text{CN}$	(Butanenitrile, 3-methyl-)	546
$(\text{CH}_3)_3\text{CCN}$	(Propanenitrile, 2,2-dimethyl-)	546
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}(\text{CH}_3)_2$	(Diazene, ethyl-(1-methylethyl)-)	546
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{NH}_2$	(2-Butanamine, 2-methyl-, or t-Amylamine)	546

C₅H_xO_yN_z-COMPOUND Reactions:

CH ₃ C(O)OCH ₂ CH ₂ CN (Propanenitrile, 3-(acetyloxy)-)	547
CH ₃ CH ₂ C(CH ₃) ₂ ONO (1,1-Dimethylpropyl nitrite)	547
(CH ₃) ₂ NC(O)OCH ₂ CH ₃ (Carbamic acid, dimethyl-, ethyl ester)	547

C₆H_x-COMPOUND Reactions:

trans-CH ₂ =CHCH=CHCH=CH ₂ (1,3,5-Hexatriene, (E)-)	547
cis-CH ₃ CH=C=C=CHCH ₃ (2,3,4-Hexatriene, (Z)-)	547
cy-CH ₂ CH ₂ CH=CHCH=CH (1,3-Cyclohexadiene)	547
cy-CH ₂ CH ₂ CH=CHCH=CH + cy-CH ₂ CH ₂ CH=CHCH=CH (1,3-Cyclohexadiene + 1,3-Cyclohexadiene)	548
CH=CCH ₂ CH ₂ CH ₂ CH ₃ (1-Hexyne)	550
CH ₃ C=CCH(CH ₃) ₂ (2-Pentyne, 4-methyl-)	550
(CH ₃) ₃ CC=CH (1-Butyne, 3,3-dimethyl-)	550
CH ₃ CH ₂ CH=CHCH=CH ₂ (1,3-Hexadiene)	551
CH ₂ =CHCH ₂ CH ₂ CH=CH ₂ (1,5-Hexadiene)	551
CH ₂ =CHCH ₂ CH ₂ CH=CD ₂ (1,5-Hexadiene-1,1-d ₂)	551
cis-CH ₃ CH=C(CH ₃)CH=CH ₂ (1,3-Pentadiene, 3-methyl-, (Z)-)	551
CH ₂ =CHCH(CH ₃)CH=CH ₂ (1,4-Pentadiene, 3-methyl-)	551
cy-C ₆ H ₁₀ (Cyclohexene)	551
cy-CH ₂ CH ₂ CH ₂ C(=CHCH ₃) (Cyclobutane, ethylidene-)	552
cy-CH ₂ CH ₂ C(=CH ₂)CH(CH ₃) (Cyclobutane, 1-methyl-2-methylene-)	552
cy-CH(CH ₃)CH ₂ C(=CH ₂)CH ₂ (Cyclobutane, 1-methyl-3-methylene-)	552
Spiro-[CH(CH ₃)CH ₂]>C<(CH ₃) ₂ (Spiropentane, methyl-)	553
CH ₂ CH ₂ CH ₂ CH ₂ CH=CH ₂ [†] (5-Hexenyl)	553
cy-(CH ₂) ₅ CH + cy-(CH ₂) ₅ CH (Cyclohexyl + Cyclohexyl)	554
cy-(CD ₂) ₅ CD + cy-(CD ₂) ₅ CD (Cyclohexyl-d ₁₁ + Cyclohexyl-d ₁₁)	554
cy-(CH ₂) ₅ CH + (cy-C ₆ H ₁₁)N=N(C ₆ H ₁₁ -cy) (Cyclohexyl + Azocyclohexane)	555
CH ₂ =CH(CH ₂) ₃ CH ₃ (1-Hexene)	555
cis-CH ₃ CH ₂ CH ₂ CH=CHCH ₃ (2-Hexene, (Z)-)	555
(CH ₃) ₂ CHC(CH ₃)=CH ₂ (1-Butene, 2,3-dimethyl-)	555
(CH ₃) ₃ CCH=CH ₂ (1-Butene, 3,3-dimethyl-)	556
cis-CH(CH ₃)CH(CH ₃)CH ₂ CH ₂ (1,4-Butanediyl, 1,2-dimethyl- (Z)-)	556
trans-CH(CH ₃)CH(CH ₃)CH ₂ CH ₂ (1,4-Butanediyl, 1,2-dimethyl-, (E)-)	556
cy-C ₆ H ₁₂ (Cyclohexane)	557
trans-cy-CH ₂ CH ₂ CH(CH ₃)CH(CH ₃) (Cyclobutane, 1,2-dimethyl-, trans-)	558
cy-C(CH ₃) ₂ CH(CH ₃)CH ₂ (Cyclopropane, 1,1,2-trimethyl-)	559
CH ₃ CHCH ₂ CH ₂ CH ₂ CH ₃ [†] (Pentyl, 1-methyl-)	560
(CH ₃) ₂ CHCH(CH ₃)CH ₂ (Butyl, 2,3-dimethyl-)	560
n-C ₆ H ₁₄ (n-Hexane)	560
(CH ₃) ₂ CHCH ₂ CH ₂ CH ₃ (Pentane, 2-methyl-)	561
(CH ₃) ₃ CCH ₂ CH ₃ (Butane, 2,2-dimethyl-)	561
(CH ₃) ₃ CCH ₂ CH ₃ [†] (Butane, 2,2-dimethyl-)	561

$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ (Butane, 2,3-dimethyl-) 561

$\text{C}_6\text{H}_x\text{O}_y$ -COMPOUND Reactions:

$\text{CH}=\text{CC}(\text{CH}_3)_2\text{COOH}$ (3-Butynoic acid, 2,2-dimethyl-)	562
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}=\text{CH}$ (3-Butyn-1-ol acetate)	562
$(\text{CH}_2=\text{CHCH}_2)_2\text{O}$ (Diallylether)	562
bicy- $\text{C}_6\text{H}_{10}\text{O}$ (1,2-Epoxycyclohexane)	562
bicy- $\text{C}_6\text{H}_6\text{D}_4\text{O}$ (7-Oxabicyclo[4.1.0]heptane-2,2,5,5- d_4)	563
$\text{CH}_2=\text{CHC}(\text{CH}_3)_2\text{COOH}$ (3-Butenoic acid, 2,2-dimethyl-)	563
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (3-Buten-1-ol acetate)	563
[cy- $\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)$] CH_2COOH (Cyclopropaneacetic acid, 1-methyl-)	563
trans-[cy- $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}$] CH_2COOH (Cyclopropaneacetic acid, 2-methyl-, trans-)	564
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (2-Butanone, 4-(acetyloxy)-)	564
$(\text{CH}_3)_2\text{CHCH}_2\text{OCH}=\text{CH}_2$ (Propane, 1-(ethenyloxy)-2-methyl-)	564
$(\text{CH}_3)_2\text{CHOC}(\text{CH}_3)=\text{CH}_2$ (1-Propene, 2-(1-methylethoxy)-)	564
$(\text{CH}_3)_3\text{COCH}=\text{CH}_2$ (Propane, 2-(ethenyloxy)-2-methyl-)	565
cy- $(\text{CH}_3)\text{C}(\text{CH}_2\text{CH}_3)\text{CH}_2\text{OCH}_2$ (Oxetane, 3-ethyl-3-methyl-)	565
cy- $\text{C}(\text{CH}_3)_2\text{C}(\text{CH}_3)_2\text{O}$ (Oxirane, tetramethyl-)	565
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (n-Butyl acetate)	565
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$ (Propanoic acid 1-methylethyl ester)	565
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$ (t-Butyl acetate)	566
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CD}_3)_3$ (t-Butyl- d_9 acetate)	566
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{OCH}_3$ (1-Propanol, 3-methoxy-, acetate)	566
$\text{CH}_3\text{OCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$ (Acetic acid, methoxy-, 1-methylethyl ester)	566
$\text{CH}_3\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_3$ (Carbonic acid ethyl propyl ester)	566
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2$ (Propoxy, 1,1,2-trimethyl-)	566
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2$ (Propoxy, 1,1,2-trimethyl-) + O_2	566
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2$ + $(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$	567
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ (Propyldioxy, 1,1,2-trimethyl-) + $(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$	567
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ + $(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$	567
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ (Propyldioxy, 1,1,2-trimethyl-)	567
$(\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2\text{OH}$ (2-Butanol, 2,3-dimethyl-)	567
$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{OH}$ (2-Butanol, 3,3-dimethyl-)	568

$\text{C}_6\text{H}_x\text{S}_y$ -COMPOUND Reactions:

$\text{CH}_2=\text{CHCH}_2\text{SCH}_2\text{CH}=\text{CH}_2$ (Diallyl sulfide)	568
$\text{CH}_3\text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2$ (1-Propene, 3-(propenylthio)-)	568

$\text{C}_6\text{H}_x\text{O}_y\text{S}_z$ -COMPOUND Reactions:

$\text{CH}_3\text{C}(\text{S})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (Ethanethioic acid O-butyl ester)	568
$\text{CH}_3\text{C}(\text{S})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (Ethanethioic acid O-(1-methylpropyl) ester)	569

CH ₃ C(S)OCH ₂ CH(CH ₃) ₂	(Ethanethioic acid O-(2-methylpropyl) ester)	569
CH ₃ C(O)SCH ₂ CH ₂ CH ₂ CH ₃	(Ethanethioic acid S-butyl ester)	569
CH ₃ C(O)SCH ₂ CH(CH ₃) ₂	(Ethanethioic acid S-(2-methylpropyl) ester)	569
CH ₃ C(O)SCH(CH ₃)CH ₂ CH ₃	(Ethanethioic acid S-(1-methylpropyl) ester)	570
CH ₃ C(O)SC(CH ₃) ₃	(Ethanethioic acid S-(1,1-dimethylethyl) ester)	570
CH ₃ OC(O)SC(CH ₃) ₃	(Carbonothioic acid S-(1,1-dimethylethyl) ester)	570
(CH ₃) ₃ COC(O)SCH ₃	(Carbonothioic acid O-(1,1-dimethylethyl) ester)	570
CH ₃ C(S)SCH ₂ CH ₂ CH ₂ CH ₃	(Ethane(dithioic) acid butyl ester)	570
CH ₃ C(S)SCH(CH ₃)CH ₂ CH ₃	(Ethane(dithioic) acid 1-methylpropyl ester)	571
CH ₃ C(S)SC(CH ₃) ₃	(Ethane(dithioic) acid 1,1-dimethylethyl ester)	571
CH ₃ OC(S)SC(CH ₃) ₃	(Carbonodithioic acid S-(1,1-dimethylethyl) ester)	571

C₆H_xN_y-COMPOUND Reactions:

trans-cy-CH ₂ CH ₂ CH(CN)CH(CN)	(1,2-Cyclobutanedicarbonitrile, trans-)	571
cy-CH ₂ C(=CH ₂)CH ₂ CH(CN)	(Cyclobutanecarbonitrile, 3-methylene-)	571
(cy-CH ₂ CH ₂ CH)N=CHCH ₂ CH ₃	(Cyclopropanamine, N-propylidene-)	..	572
cy-CH(CH ₂ CH ₃)CH ₂ CH ₂ CH=N	(2H-Pyrrole, 2-ethyl-3,4-dihydro-)	..	572
CH ₂ =CHCH ₂ NHCH ₂ CH=CH ₂	(2-Propen-1-amine, N-(2-propenyl)-)	572
(CH ₃) ₂ CHN=NCH ₂ CH=CH ₂	(Diazene, (1-methylethyl)-2-propenyl-)	.	572
CH ₃ CH ₂ CH ₂ N=NCH ₂ CH ₂ CH ₃ *	(Azo-n-propane)	573
(CH ₃) ₂ CHN=NCH(CH ₃) ₂	(Azoisopropane)	573
(CH ₃) ₂ CHN=NCH(CH ₃) ₂ *	(Azoisopropane)	573

C₆H_xO_yN_z-COMPOUND Reactions:

CH ₃ CONHC(CH ₃) ₃	(Acetamide, N-(1,1-dimethylethyl)-) (+ M)	574
CH ₃ C(O)OC(CH ₃) ₂ CN	(Propanenitrile, 2-(acetyloxy)-2-methyl-)	.	574
CH ₃ C(O)OCH ₂ CH ₂ N(CH ₃) ₂	(Acetic acid 2-(dimethylamino)ethyl ester)	574
(CH ₃) ₂ NC(O)OCH(CH ₃) ₂	(Carbamic acid, dimethyl-, 1-methylethyl ester)	574

C₇H_x-COMPOUND Reactions:

CH=CCH ₂ CH ₂ CH ₂ C=CH	(1,6-Heptadiyne)	574
CH ₂ =C=CHCH(CH ₃)C≡CH	(1,2-Hexadien-5-yne, 4-methyl-)	574
cy-CH=CHCH=CHCH=CHCH ₂	(1,3,5-Cycloheptatriene)	575

bicy-C ₇ H ₈ (Bicyclo[2.2.1]hepta-2,5-diene; 2,5-Norbornadiene)	575
bicy-C ₇ H ₁₀ (Bicyclo[2.2.1]hept-2-ene; Norbornene)	575
bicy-C ₇ H ₁₀ (Bicyclo[3.2.0]hept-2-ene)	576
tricy-C ₆ H ₁₀ (Tricyclo[4.1.1.0 ^{1,3}]heptane)	576
CH=CCH ₂ CH(CH ₃)CH ₂ CH ₃ (1-Hexyne, 4-methyl-)	577
CH=CCH ₂ CH ₂ CH(CH ₃) ₂ (1-Hexyne, 5-methyl-)	577
CH ₃ C=CC(CH ₃) ₃ (2-Pentyne, 4,4-dimethyl-)	577
CH ₂ =CHCH ₂ CH ₂ CH ₂ CH=CH ₂ (1,6-Heptadiene)	578
cis-CH ₂ =C(CH ₃)C(CH ₃)=CHCH ₃ (1,3-Pentadiene, 2,3-dimethyl-, (Z)-)	578
trans-CH ₂ =C(CH ₃)C(CH ₃)=CHCH ₃ (1,3-Pentadiene, 2,3-dimethyl-, (E)-)	578
CH ₂ =CHC(CH ₃)=C(CH ₃) ₂ (1,3-Pentadiene, 3,4-dimethyl-)	578
cy-(CH ₂) ₄ CH=C(CH ₃) (Cyclohexene, 1-methyl-)	579
(-)-C(CH ₂ CH ₃)=CHCH(CH ₂ CH ₃) (Cyclopropene, 1,3-diethyl-, (-)-)	579
(+)-C(CH ₂ CH ₃)=CHCH(CH ₂ CH ₃) (Cyclopropene, 1,3-diethyl-, (+)-)	580
bicy-C ₇ H ₁₂ (Bicyclo[4.1.0]heptane)	580
CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ (1-Heptene)	581
cis-CH ₃ CH ₂ CH ₂ CH ₂ CH=CHCH ₃ (2-Heptene, (Z)-)	581
(CH ₃) ₂ CHCH=C(CH ₃) ₂ (2-Pentene, 2,4-dimethyl-)	581
cy-C(CH ₃) ₂ CH(CH ₃)CH ₂ CH ₂ (Cyclobutane, 1,1,2-trimethyl-)	581
cy-C(CH ₃) ₂ C(CH ₃) ₂ CH ₂ (Cyclopropane, 1,1,2,2-tetramethyl-)	582
(CH ₃) ₂ CHCH ₂ C(CH ₃) ₂ [†] (Butyl, 1,1,3-trimethyl-)	582
(CH ₃) ₃ CCH ₂ CHCH ₃ [†] (Butyl, 1,3,3-trimethyl-)	582
(CH ₃) ₂ CHC(CH ₃) ₂ CH ₂ (Butyl, 2,2,3-trimethyl-)	582
(CH ₃) ₃ CCH(CH ₃)CH ₂ (Butyl, 2,3,3-trimethyl-)	582
(CH ₃) ₃ CC(CH ₃) ₂ (Propyl, 1,1,2,2-tetramethyl-)	583
(CH ₃) ₃ CC(CH ₃) ₂ + O ₂	583
n-C ₇ H ₁₆ (n-Heptane)	584
(CH ₃) ₂ CHCH ₂ CH(CH ₃) ₂ (Pentane, 2,4-dimethyl-)	584
(CH ₃) ₃ CCH(CH ₃) ₂ (Butane, 2,2,3-trimethyl-)	584

C₇H_xO_y-COMPOUND Reactions:

bicy-C ₇ H ₈ O (Bicyclo[3.2.0]hept-2-en-6-one)	584
bicy-C ₇ H ₁₀ O (Bicyclo[3.2.0]heptan-6-one)	584
CH ₂ =C=CHC(CH ₃) ₂ COOH (3,4-Pentadienoic acid, 2,2-dimethyl-)	584
CH ₂ =C(CH ₃)C(CH ₃) ₂ COOH (3-Butenoic acid, 2,2,3-trimethyl-)	585
CH ₃ C(O)OCH ₂ CH ₂ CH ₂ CH=CH ₂ (4-Penten-1-ol acetate)	585
CH ₃ C(O)OCH(CH ₃)CH ₂ CH=CH ₂ (4-Penten-2-ol acetate)	585
trans-CH ₃ CH=CHCOOCH(CH ₃) ₂ (2-Butenoic acid, (E)-, 1-methylethyl ester)	585
[cy-(CH ₂) ₅ CH]OC(O)H (Cyclohexyl formate)	585
[cy-(CH ₂) ₄ CH]OC(O)CH ₃ (Cyclopentanol acetate)	585
(cy-CH ₂ CH ₂ CH)C(CH ₃) ₂ COOH (Cyclopropaneacetic acid, α,α-dimethyl-)	586
[cy-CH ₂ C(CH ₃) ₂ CH]CH ₂ COOH (Cyclopropaneacetic acid, 2,2-dimethyl-)	586
CH ₃ C(O)OCH ₂ CH ₂ CH ₂ COCH ₃ (2-Pentanone, 5-acetyloxy-)	586

$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{COCH}_3$	(2-Butanone, 3-(acetyloxy)-3-methyl-)	.. 587
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{C}(\text{O})\text{OCH}_3$	(Propanoic acid, 2-(acetyloxy)- 2-methyl-, methyl ester) 587
cy- $\text{CH}_2\text{C}(\text{CH}_2\text{CH}_3)_2\text{CH}_2\text{O}$	(Oxetane, 3,3-diethyl-) 587
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$	(1-Butanol, 3-methyl-, acetate) 587
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2 + \text{O}_2(\text{a}^1\Delta_g)$	 587
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}_3$	(2-Butanol, 2-methyl-, acetate) 587
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$	(2-Butanol, 3-methyl-, acetate) 588
$(\text{CH}_3)_2\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Propanoic acid, 2-methyl-, 1-methyl ethyl ester) 588
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$	(Propanoic acid 1,1-dimethylethyl ester)	. 588
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Butanoic acid 1-methylethyl ester)	.. 588
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_3$	(Carbonic acid dipropyl ester) 588
$(\text{CH}_3)_2\text{CHOC}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Carbonic acid bis(1-methylethyl) ester) 588
$(\text{CD}_3)_2\text{CHOC}(\text{O})\text{OCH}(\text{CD}_3)_2$	(Carbonic acid bis(1-methyl-d ₃ - ethyl-2,2,2-d ₃) ester) 589
$\text{CH}_3\text{OCH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$	(Acetic acid, methoxy-, 1,1-dimethylethyl ester) 589
$\text{CH}_3\text{OC}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}_3$	(Carbonic acid 1,1-dimethylpropyl methyl ester) 589
$\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OOH}$	(Hydroperoxide, heptyl-) 589
$\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{OOH})\text{CH}_3$	(Hydroperoxide, 1-methylhexyl-) 590

$\text{C}_7\text{H}_x\text{S}_y$ -COMPOUND Reactions:

$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2$	(Butane, 1-(2-propenylthio)-) 590
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$\text{C}_7\text{H}_x\text{N}_y$ -COMPOUND Reactions:

$(\text{CH}_3)_3\text{CN}=\text{NCH}_2\text{CH}=\text{CH}_2$	(Diazene, (1,1-dimethylethyl)-2-propenyl)	590
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$\text{C}_7\text{H}_x\text{O}_y\text{N}_z$ -COMPOUND Reactions:

$(\text{CH}_3)_2\text{NC}(\text{O})\text{OC}(\text{CH}_3)_3$	(Carbamic acid, dimethyl-, 1,1-dimethylethyl ester) 590
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OC}(\text{CD}_3)_3$	(Carbamic acid, dimethyl-, (1,1-dimethyl-d ₉) ester) 590

C_8H_x -COMPOUND Reactions:

cy- $\text{CH}=\text{CHCH}=\text{CHC}(\text{=CH}_2)\text{C}(\text{=CH}_2)$	(1,3-Cyclohexadiene, 5,6-bis(methylene)-) 591
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}=\text{C}=\text{CH}_2$	(1,2,6,7-Octatetraene) 591
$\text{CH}_2=\text{CHC}(\text{=CH}_2)\text{C}(\text{=CH}_2)\text{CH}=\text{CH}_2$	(1,5-Hexadiene, 3,4-bis(methylene)-) 591
cy- $\text{C}(\text{CH}=\text{CH}_2)\text{C}(\text{CH}=\text{CH}_2)\text{CH}_2\text{CH}_2$	(Cyclobutene, 1,2-diethenyl-)	... 591
cy- $\text{CHC}(\text{=CH}_2)\text{C}(\text{=CH}_2)\text{CHCH}_2\text{CH}_2$	(1,4-Cyclohexanediyl, 2,3-bis(methylene)-) 592

bicy-C ₈ H ₁₀ (Bicyclo[4.2.0]octa-1,5-diene)	592
bicy-C ₈ H ₁₀ (Bicyclo[2.2.0]hexane, 2,3-bis(methylene)-)	592
bicy-C ₈ H ₁₀ (Bicyclo[2.2.2]octa-2,5-diene)	593
trans,trans,trans-CH ₃ CH=CHCH=CHCH=CHCH ₃ (2,4,6-Octatriene, (E,E,E)-)	593
cis,cis-cy-CH=CHCH ₂ CH ₂ CH=CHCH ₂ CH ₂ (1,5-Cyclooctadiene, (Z,Z)-)	593
cy-CH=CHCH ₂ CH(CH=CH ₂)CH ₂ CH ₂ (Cyclohexene, 4-ethenyl-)	594
(+)-cy-CH=CHCH ₂ CH(CH=CD ₂)CH ₂ CH ₂ (Cyclohexene, 4-(ethenyl-2,2-d ₂)-, (R)-)	594
cy-C(CH ₂ CH ₃)=CHCH ₂ CH=CHCH ₂ (1,4-Cyclohexadiene, 1-ethyl-) ...	595
cy-C(CH ₃)=C(CH ₃)CH ₂ CH=CHCH ₂ (1,4-Cyclohexadiene, 1,2-dimethyl-)	595
trans-cy-CH(CH=CH ₂)CH(CH=CH ₂)CH ₂ CH ₂ (Cyclobutane, 1,2-diethenyl, trans-)	595
cis-cy-CH(CH ₃)CH(CH ₃)C(=CH ₂)C(=CH ₂) (Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, cis-)	595
trans-cy-CH(CH ₃)CH(CH ₃)C(=CH ₂)C(=CH ₂) (Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, trans-) ...	596
bicy-C ₈ H ₁₂ (Bicyclo[2.2.2]oct-2-ene)	596
CH ₃ C≡CCH ₂ CH ₂ CH(CH ₃) ₂ (2-Heptyne, 6-methyl-)	596
CH ₃ CH ₂ CH(CH ₃)CH ₂ C(CH ₃)=CH ₂ (1-Hexene, 2,4-dimethyl-)	597
(CH ₃) ₃ CC(CH ₃) ₂ CH ₂ (Butyl, 2,2,3,3-tetramethyl-)	597
n-C ₈ H ₁₈ (n-Octane)	597
(CH ₃) ₂ CH(CH ₂) ₄ CH ₃ (Heptane, 2-methyl-)	597
(CH ₃) ₃ CC(CH ₃) ₃ (Hexamethylethane)	598

C₈H_xO_y-COMPOUND Reactions:

bicy-C ₈ H ₁₀ O (Bicyclo[3.2.0]hept-3-en-6-one, 5-methyl-)	599
CH ₂ CH=CH ₂ OC(O)C(O)OCH ₂ CH=CH ₂ (Ethanedioic acid di-2-propenyl ester)	599
CH ₂ =CHCH=CHC(CH ₃) ₂ COOH (3,5-Hexanedioic acid, 2,2-dimethyl-)	599
CH ₂ =CHCH=CHC(CH ₃) ₂ COOD (3,5-Hexanedioic acid-d, 2,2-dimethyl-)	599
(cy-CH ₂ CH ₂ CH=CHCH ₂ CH)OC(O)CH ₃ (3-Cyclohexen-1-ol acetate) ...	599
CH ₃ C(O)OCH ₂ CH ₂ CH ₂ CH ₂ CH=CH ₂ (5-Hexen-1-ol acetate)	600
CH ₃ C(O)OCH ₂ CH ₂ CH=C(CH ₃) ₂ (3-Penten-1-ol, 4-methyl-, acetate)	600
CH ₃ C(O)OC(CH ₃) ₂ CH ₂ CH=CH ₂ (4-Penten-2-ol, 2-methyl-, acetate)	600
(cy-C ₆ H ₁₁)OC(O)CH ₃ (Acetic acid cyclohexyl ester)	600
bicy-C ₈ H ₁₄ O (Cyclobutanone, 3-ethoxy-2,2-dimethyl-)	600
[cy-CH ₂ CH ₂ C(CH ₃)]C(CH ₃) ₂ COOH (Cyclopropaneacetic acid, α,α,1-trimethyl)	601
cis-syn-[cy-CH(CH ₃)CH(CH ₃)CH]C(O)OCH ₃ (Cyclopropanecarboxylic acid, 2,3-dimethyl-, ethyl ester, (1α,2α,3α)-)	601
trans-[cy-CH(CH ₃)CH(CH ₃)CH]C(O)OCH ₃ (Cyclopropanecarboxylic acid, 2,3-dimethyl-, ethyl ester, (1α,2α,3β)-)	601
CH ₃ C(O)OC(CH ₃) ₂ CH ₂ COCH ₃ (2-Pentanone, 4-(acetyloxy)-4-methyl-)	601
CH ₃ CH ₂ CH ₂ CH ₂ C(O)OCH(CH ₃) ₂ (Pentanoic acid 1-methylethyl ester)	601
CH ₃ C(O)OCH ₂ CH ₂ C(CH ₃) ₃ (1-Butanol, 3,3-dimethyl-, acetate) ...	602
CH ₃ C(O)OCH(CH ₃)C(CH ₃) ₃ (2-Butanol, 3,3-dimethyl-, acetate) ..	602

$(\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Butanoic acid, 3-methyl-, 1-methylethyl ester) 602
$(\text{CH}_3)_3\text{CC}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Propanoic acid, 2,2-dimethyl-, 1-methylethyl ester) 602
$\text{CH}_3\text{OC}(\text{O})\text{O}(\text{CH}_2)_5\text{CH}_3$	(Carbonic acid hexyl methyl ester) 602
$\text{CH}_3\text{OC}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	(Carbonic acid methyl 1-methylpentyl ester) 602
$(\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3$	(Peroxide, bis(1,1-dimethylethyl)-) 603

$\text{C}_8\text{H}_x\text{S}_y$ -COMPOUND Reactions:

$(\text{CH}_3)_3\text{CSC}(\text{CH}_3)_3$	(Propane, 2,2'-thiobis[2-methyl-]) 603
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$\text{C}_8\text{H}_x\text{N}_y$ -COMPOUND Reactions:

$(\text{CH}_3)_2\text{CHCH}_2\text{N}=\text{NCH}_2\text{CH}(\text{CH}_3)_2$	(Diazene, bis(2-methylpropyl)-)	... 603
$(\text{CH}_3)_3\text{CN}=\text{NC}(\text{CH}_3)_3$	(Diazene, bis(1,1-dimethylethyl)-) 603

C_9 -COMPOUND Reactions:

bicy- C_9H_{12}	(1H-Indene, 2,3,4,7-tetrahydro-) 604
exo-bicy- C_9H_{14}	(Bicyclo[2.2.2]oct-2-ene, 5-methyl-, (1 α ,4 α ,5 α)-) 604
endo-bicy- C_9H_{14}	(Bicyclo[2.2.2]oct-2-ene, 5-methyl-, (1 α ,4 α ,5 β)-) 604
bicy- $\text{C}_9\text{H}_8\text{O}$	(o-Quinodimethane) 605
bicy- $\text{C}_9\text{H}_{12}\text{O}$	(Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, (1 α ,2 β ,4 α)-) 605
bicy- $\text{C}_9\text{H}_{12}\text{O}$	(Bicyclo[3.2.0]hept-2-en-6-one, 7,7-dimethyl-) 605
trans-[cy-CH(CH ₃)(CH ₂) ₄ CH]OC(O)CH ₃	(Cyclohexanol, 2-methyl-, acetate, (1R-trans)-) 605
cis-[cy-CH(CH ₃)(CH ₂) ₄ CH]OC(O)CH ₃	(Cyclohexanol, 2-methyl-, acetate, (1S-cis)-) 606
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}(\text{CH}_3)_2$	(2-Pentanol, 2,4-dimethyl-, acetate) 606
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{C}(\text{CH}_3)_3$	(2-Pentanol, 4,4-dimethyl-, acetate)	606
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_2\text{CH}_3)\text{C}(\text{CH}_3)_3$	(3-Pentanol, 2,2-dimethyl-, acetate)	606
$\text{CH}_3\text{C}(\text{O})\text{OC}[\text{CH}(\text{CH}_3)_2](\text{CH}_3)\text{CH}_2\text{CH}_3$	(3-Pentanol, 2,3-dimethyl-, acetate) 607
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{C}(\text{CH}_3)_3$	(2-Butanol, 2,3,3-trimethyl-, acetate)	607
$(\text{CH}_3)_3\text{CC}(\text{O})\text{OC}(\text{CH}_3)_3$	(Propanoic acid, 2,2-dimethyl-, 1,1-dimethylethyl ester) 607
$(\text{CH}_3\text{CH}_2)_2\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Butanoic acid, 2-ethyl-, 1-methylethyl ester) 607
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Butanoic acid, 3,3-dimethyl-, 1-methylethyl ester) 607
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$	(Pentanoic acid, 2-methyl-, 1-methylethyl ester) 607

CH ₃ (CH ₂) ₄ C(O)OCH(CH ₃) ₂ (Hexanoic acid 1-methylethyl ester)	..	607
CH ₃ CH ₂ CH ₂ CH ₂ OC(O)OCH ₂ CH ₂ CH ₂ CH ₃ (Carbonic acid dibutyl ester)		607
CH ₃ CH ₂ CH(CH ₃)OC(O)OCH(CH ₃)CH ₂ CH ₃ (Carbonic acid bis(1-methylpropyl) ester)	608
(CH ₃) ₂ CHCH ₂ OC(O)OCH ₂ CH(CH ₃) ₂ (Carbonic acid bis(2-methylpropyl) ester)	608
(CH ₃) ₃ COC(O)OC(CH ₃) ₃ (Carbonic acid bis(1,1-dimethylethyl) ester)	608
(CH ₂ =CHCH ₂) ₃ N (Triallylamine)	609
[cy-(CH ₂) ₅ CH]NHCH ₂ CH=CH ₂ (Cyclohexanimine, N-2-propenyl-)	...	609

C₁₀ to C₁₅-COMPOUND Reactions:

(cy-CH=CHCH ₂ CH ₂ C)=(CCH ₂ CH ₂ CH=CH-cy) (Cyclopentene, 3-(4-Cyclopenten-1-ylidene)- (trans form))	609
anti-cis-tricy-C ₁₀ H ₁₂ (Tricyclo[5.3.0.0 ^{2,6}]deca-3,9-diene; anti-cis-[2+2]-Dicyclopentadiene)	609
endo-tricy-C ₁₀ H ₁₂ (Tricyclo[5.2.1.0 ^{2,6}]deca-3,8-diene, endo-)		610
exo-tricy-C ₁₀ H ₁₂ (-tricy-clo[5.2.1.0 ^{2,6}]deca-3,8-diene, exo-)		610
anti-tricy-C ₁₀ H ₁₂ (Tricyclo[4.2.1.1 ^{2,5}]deca-3,7-diene, (1 α , 2 β , 5 β , 6 α)-)	610
CH ₂ =C=CHCH ₂ CH ₂ CH ₂ CH ₂ CH=C=CH ₂ (1,2,8,9-Decatetraene)	611
bicy-C ₁₀ H ₁₄ (Bicyclo[4.2.2]deca-3,7-diene)	611
bicy-C ₁₀ H ₁₄ (Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α , 4 α , 5 α)-)	612
bicy-C ₁₀ H ₁₄ (Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α , 4 α , 5 β)-)	613
n-C ₁₀ H ₂₂ (n-Decane)	613
(bicy-C ₆ H ₉)C(CH ₃) ₂ COOH (Bicyclo[3.1.0]hexane-1-acetic acid, α , α -dimethyl-)	614
trans-cy-(CH ₂) ₄ CH[OC(O)CH ₃]CH[OC(O)CH ₃] (1,2-Cyclohexanediol diacetate, trans-)	615
cis-cy-(CH ₂) ₄ CH[OC(O)CH ₃]CH[OC(O)CH ₃] (1,2-Cyclohexanediol diacetate, cis-)	615
CH ₃ COOCH[C(CH ₃) ₃]CH ₂ CH=CH ₂ (5-Hexen-3-ol, 2,2-dimethyl-, acetate)	615
[cy-CH ₂ CH(CH ₃)C(CH ₂ CH ₃)]C(CH ₃) ₂ COOH (Cyclopropaneacetic acid, 1-ethyl- α , α ,2-trimethyl-)	616
CH ₃ COOCH[CH(CH ₃) ₂]C(CH ₃) ₃ (3-Pentanol, 2,2,4-trimethyl-, acetate)	616
(CH ₃) ₃ CCH ₂ COOC(CH ₃) ₃ (Butanoic acid, 3,3-dimethyl-, 1,1-dimethylethyl ester)	616
C ₆ H ₅ CH ₂ SCH ₂ CH=CH ₂ (Benzene, [(2-propenylthio)methyl]-; Allyl benzyl sulfide)	616
(bicy-C ₇ H ₁₁)C(CH ₃) ₂ COOH (Bicyclo[4.1.0]heptane-1-acetic acid, α , α -dimethyl-)	617
endo-tricy-C ₁₂ H ₁₆ (endo-Tricyclo[6.2.2.0 ^{2,7}]dodeca-3,9-diene)		617
n-C ₁₂ H ₂₆ (n-Dodecane)	617

[cy-(CH ₂) ₆ CH=C]C(CH ₃) ₂ COOH	(1-Cyclooctene-1-acetic acid, α,α-dimethyl-)	618
(CH ₃) ₂ CC(O)O[CH(CH ₂) ₅ -cy]	(Propanoic acid, 2,2-dimethyl-, cyclohexyl ester)	618
CH ₃ CH ₂ C(CH ₃) ₂ OOC(CH ₃) ₂ CH ₂ CH ₃	(Peroxide, bis(1,1-dimethylpropyl)-)	618
(CH ₃ CH ₂ CH ₂) ₂ CHCOOCH(CH ₃) ₂	(Pentanoic acid, 2-propyl-, 1-methylethyl ester)	618
CH ₃ CH ₂ C(CH ₃) ₂ OCOOC(CH ₃) ₂ CH ₂ CH ₃	(Carbonic acid bis(1,1-dimethylpropyl) ester)	618
trans-cy-(CH ₂) ₄ CH[OC(O)CH ₃]CH[C(CH ₃) ₃]	(Cyclohexanol, 2-(1,1-dimethylethyl)-acetate, trans-)	619
cis-cy-(CH ₂) ₄ CH[OC(O)CH ₃]CH[C(CH ₃) ₃]	(Cyclohexanol, 2-(1,1-dimethylethyl)-acetate, cis-)	619
trans-cy-(CH ₂) ₂ CH[OC(O)CH ₃](CH ₂) ₂ CH[C(CH ₃) ₃]	(Cyclohexanol, 4-(1,1-dimethylethyl)-acetate, trans-)	620
cis-cy-(CH ₂) ₂ CH[OC(O)CH ₃](CH ₂) ₂ CH[C(CH ₃) ₃]	(Cyclohexanol, 4-(1,1-dimethylethyl)-acetate, cis-)	620
CH ₃ C(O)O[CH(CH ₃) ₂ CH ₂ CH ₂ CH(CH ₃)CH ₂ -cy]	(Cyclohexanol, 5-methyl- 2-(1-methylethyl)-acetate, (1α,2β,5β)-)	621
(bicy-C ₈ H ₁₃)C(CH ₃) ₂ COOH	(Bicyclo[5.1.0]octane-1-acetic acid, α,α-dimethyl-)	621
(bicy-C ₉ H ₁₅)C(CH ₃) ₂ COOH	(Bicyclo[6.1.0]nonane-1-acetic acid, α,α-dimethyl-)	622
CH ₃ (CH ₂) ₅ OC(O)O(CH ₂) ₅ CH ₃	(Carbonic acid dihexyl ester)	623
CH ₃ (CH ₂) ₃ CH(CH ₃)OC(O)OCH(CH ₃)(CH ₂) ₃ CH ₃	(Carbonic acid bis(1-methylpentyl) ester)	623
CH ₃ (CH ₂) ₅ CH ₂ OOCH ₂ (CH ₂) ₅ CH ₃	(Peroxide, diheptyl-)	623
n-C ₁₅ H ₃₂	(n-Pentadecane)	623

4. Table of Chemical Kinetic Data for Combustion Chemistry

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + O + O → O₂ + O(¹S)						
Oxygen atom						
76 SLA/BLA1	EX	200-302	5.08(17)	0	654±302	3 3.07
O + O (+ M) → O₂ (+ M)						
Oxygen atom						
72 TCH	EX	298	3.63(15)			3
M = O ₂ .						
Room temperature, assumed to be 298 K.						
73 CAM/GRA ¹⁾	EX	196	(1.74±0.13)(15)			3
73 CAM/GRA ¹⁾	EX	298	(4.05±0.17)(15)			3
¹⁾ M = N ₂ .						
O + O₂ + O₂ → O₃ + O₂(¹Δ_g)						
Oxygen atom + Oxygen molecule						
71 FIN/SNE	DE	283-321	3.16(11)	0	1681	3
k ₁ = k ₋₁ K.						
O + O₂ (+ M) → O₃ (+ M)						
Oxygen atom + Oxygen molecule						
71 ELL/CAS	RL	298	5.5(-3)			2/2
M = He, Ar, Xe, N ₂ (at 253.7nm.)						
k _{ref} : O + O ₃ → O ₂ + O ₂ .						
71 HIP/TRO	EX	298	1.0(12)			2 1.2
Limiting high-pressure k.						
72 CAS/SCH ¹⁾	RL	261	2.67(-2)			2/2
72 CAS/SCH ¹⁾	RL	298	5.5(-3)			2/2
¹⁾ M = O ₂ , O ₃ , N ₂ (at 334 nm.)						
k _{ref} : O + O ₃ → O ₂ + O ₂ .						
73 STE/NIK1	RL	298	(1.08±0.12)(-3)			2/2
M = N ₂ + O ₂ . k _{ref} : O + NO ₂ → O ₂ + NO.						
The rate ratio is given by the expression						
k[M]/k _{ref} , therefore it is dimensionless.						
73 CAS/SCH ²⁾	RL	261	2.67(-2)			2/2
73 CAS/SCH ²⁾	RL	298	5.5(-3)			2/2
²⁾ M = O ₂ , N ₂ (at 334 nm.)						
k _{ref} : O + O ₃ → O ₂ + O ₂ .						
73 GAE/GLA	RN	300	6.0(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 GAE/TRO M = N ₂ . Limiting high-pressure k. Reevaluation.	EX	296	(1.7±0.7)(12)			2	
75 HIP/SCH Limiting high-pressure k.	RN	295	(1.7±0.7)(12)			2	
71 HIP/TRO M = N ₂ . Low-pressure k. Rate constant expressed as: k/[N ₂].	EX	298	2.9(14)			3	1.2
71 PRA/KAR O ₂ Photolysis. P(M) = (3-5) torr. k _{ref} : O + O ₂ + O ₂ → O ₃ + O ₂ . Efficiencies for the rate ratio are: 1.0(O ₂), (0.6±0.2)(Ar or He), (0.8±0.2)(Xe), (1.1±0.2)(N ₂), (3.2±0.5)(CO ₂).	RL	293	1.0			3/3	
71 PRA/MAK M = CO. Photolysis of O ₂ + CO mixture. P(O ₂) = 40 Tor. P(CO) = (1-60) torr. k _{ref} : O + CO → CO ₂ .	RL	293	(2.17±0.42)(7)			3/2	
71 STU/NIK1 M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 1.19(O ₂), 1.24(CO).	EX	300	2.00(14)			3	1.25
72 TCH M = O ₂ . Room temperature, assumed to be 298 K.	EX	298	4.35(14)			3	
72 HUI/HER1 M = Ar.	EX	200-346	(2.38±0.21)(13)	0	-510±23	3	
72 HUI/HER1 M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.7(N ₂).	EX	218	2.57(14)			3	
72 HUI/HER1 M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.92(He), 1.6(N ₂).	EX	298	1.32(14)			3	
73 BAL/LAR M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), Ar(0.78), 1.09(O ₂).	EX	295	(1.97±0.42)(14)			3	
73 BAL/LAR Average of present results and all the previous data. M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), Ar(0.68), 0.94(O ₂).	SE	295	(2.10±0.28)(14)			3	
73 BEV/JOH M = O ₂ . M-efficiencies relative to O ₂ are: 1.00(O ₂), 0.50(Ar), 2.41(N ₂), 2.46(CO ₂), 5.74(SF ₆).	EX	295	(1.96±0.11)(14)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 ROS/TRA M = O ₂ , or N ₂ . k _{ref} : O ₃ [†] + M → O ₃ + M.	RL	300	9.03(3)				3/2
74 ROS/TRA M = O ₂ , or N ₂ . Limiting high-pressure k.	EX	300	(1.14±0.20)(14)				3
74 SNE M = O ₂ .	EX	295	(1.8±0.18)(14)				3
75 HIP/SCH Limiting low-pressure k. Rate constant expressed as k/[N ₂]. M = N ₂ . Reevaluation.	RN	295	(2.3±1.0)(14)				3
76 HOG/BUR M = O ₂ . Computer fit of data.	DE	300	(2.27±0.34)(14)				3
77 ARE/SAM Discharge flow. M = O ₂ .	EX	298	1.20(14)				3
79 ARN/COM ³⁾ M = Ar.	EX	263-298	(2.26±0.56)(13)	0	-525±70		3
79 ARN/COM ³⁾ M = O ₂ .	EX	262-318	(2.45±0.16)(13)	0	-635±18		3
79 ARN/COM ³⁾ M = N ₂ .	EX	263-309	(6.60±0.83)(12)	0	-995±37		3
³⁾ O ₃ laser-pulse-photolysis. Resonance- absorption.							
80 KLA/AND ⁴⁾ M = O ₂ . n = 0 assumed.	EX	219-368	7.80(13)	0	-345±60		3
80 KLA/AND ⁴⁾ M = O ₂ .	EX	219-368	(2.53±0.36)(14)	-1.25	0		3
80 KLA/AND ⁴⁾ M = O ₂ .	EX	298	2.47(14)				3 1.15
80 KLA/AND ⁴⁾ M = N ₂ . n = 0 assumed.	EX	219-368	3.20(13)	0	-575±60		3
80 KLA/AND ⁴⁾ M = N ₂ .	EX	219-368	(2.28±0.33)(14)	-2.0	0		3
80 KLA/AND ⁴⁾ M = N ₂ .	EX	298	2.21(14)				3 1.15
80 KLA/AND ⁴⁾ M = Ar. n = 0 assumed.	EX	219-368	2.29(13)	0	-535±70		3
80 KLA/AND ⁴⁾ M = Ar.	EX	219-368	(1.43±0.18)(14)	-1.9	0		3
80 KLA/AND ⁴⁾ M = Ar.	EX	298	1.38(14)				3 1.15
80 KLA/AND ⁴⁾ M = Air. n = 0 assumed.	EX	219-368	3.38(13)	0	-525±60		3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 KLA/AND ⁴) M = Air.	EX	219-368	(2.31±0.34)(14)	-1.9	0	3	
80 KLA/AND ⁴) M = Air.	EX	298	2.25(14)			3	1.15
⁴) Flash-photolysis. Resonance-fluorescence. Arrhenius preexponential factor expressed as P(T/298) ⁿ in all the expressions with n ≠ 0.							
80 LAL/VER M = Ar. Pulsed photolysis of an O ₂ /Ar mixture. Resonance-fluorescence. P = 1 torr.	EX	298	(2.36±0.73)(14)			3	
80 SUG/ISH1 M = He. Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(9.07±1.08)(13)			3	
82 LIN/LEU ⁵) M = N ₂ . n = 0 assumed.	EX	218-366	(1.75±0.43)(13)	0	-731±67	3	
82 LIN/LEU ⁵) M = N ₂ .	EX	218-366	(2.11±0.07)(14)	-2.62	0	3	
82 LIN/LEU ⁵) M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.99(O ₂), 0.69(Ar), 0.60(He).	EX	298	(2.09±0.09)(14)			3	
82 LIN/LEU ⁵) M = O ₂ . n = 0 assumed.	EX	227-353	(2.27±0.38)(13)	0	-668±46	3	
82 LIN/LEU ⁵) M = O ₂ .	EX	227-353	(2.20±0.13)(14)	-2.37	0	3	
82 LIN/LEU ⁵) M = Ar. n = 0 assumed.	EX	220-353	(1.29±0.50)(13)	0	-703±102	3	
82 LIN/LEU ⁵) M = Ar.	EX	220-353	(1.41±0.10)(14)	-2.54	0	3	
⁵) Flash-photolysis. Resonance-fluorescence. Arrhenius preexponential factor expressed as (T/298) ⁿ in all the expressions with n ≠ 0.							
O + O₃ → O₂ + O₂							
Oxygen atom + Ozone							
71 KRE/SIM k _{ref} : O + COS → SO + CO.	RL	197-299	6.4(-1)	0	-101	2/2	
71 KRE/SIM	RN	197-299	7.23(12)	0	2164±101	2	
72 BAL/EGO	EX	292-370	7.07(12)	0	1933±86	2	1.29
72 HUS/KIR1	RN	300	(7.83±3.01)(9)			2	
72 MCC/KAU	EX	269-409	(6.32±1.08)(12)	0	2169±50	2	
72 MCC/KAU	EX	298	(4.52±0.36)(9)			2	
73 DAV/WON	EX	220-353	(1.22±0.11)(13)	0	2276±106	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 DAV	EX	293	(7.23±0.12)(9)			2
77 SHA	ES	250-2000	1.33(12)	0.75	1575	2
The Arrhenius preexponential factor expressed as $A(T/298)^{0.75}$.						
78 WES/WES	EX	298	≤9.03(12)			2
Resonance fluorescence. Upper-limit k. O ₃ is in the vibrational symmetric and asymmetric stretching modes: O ₃ (100,001). P = (0-100) torr.						
79 ARN/COM	EX	262-335	(1.28±0.11)(13)	0	2337±26	2
O ₃ laser-pulse-photolysis. Resonance-absorption.						
80 TOB/ULL	RL	348-433	1.0(4)	0	1610±7055	2/2 39.8
M = CO ₂ . Conventional vacuum system. P < 1.0x10 ⁻⁵ torr.						
$O(^1D) + O_3 \rightarrow O_2 + O_2$ (or $O + O + O_2$)						
Oxygen atom + Ozone						
71 GOL/GRE ¹)	RL	298	(4.1±0.9)			2/2
At 228.8 nm.						
71 GOL/GRE ¹)	RL	298	(2.6±0.4)			2/2
At 253.7 nm.						
¹) k _{ref} : $O(^1D) + N_2O \rightarrow N_2 + O_2$ (a) → NO + NO (b)						
72 LIS/HEI ²)	RL	298	(1.25±0.41)(1)			2/2
k _{ref} : $O(^1D) + N_2 \rightarrow O(^3P) + N_2$. At 228.8, or 280.0 nm.						
72 LIS/HEI ²)	RL	298	(9.09±2.02)			2/2
k _{ref} : $O(^1D) + N_2 \rightarrow O(^3P) + N_2$. At 253.7 nm.						
72 LIS/HEI ²)	RL	298	(2.50±0.83)			2/2
k _{ref} : $O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$ At 228.8, or 253.7 nm.						
72 LIS/HEI ²)	RL	298	(2.0±0.5)			2/2
k _{ref} : $O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$. At 280 nm.						
²) O ₃ Photolysis. From the reported reverse rate ratios.						
73 HEI/HUS1	EX	300	(1.62±0.12)(14)			2
73 HEI/HUS1	RL	300	3.9			2/2
k _{ref} : $O(^1D) + O_2 \rightarrow$ products.						
73 HEI/HUS3	EX	300	(1.63±0.12)(14)			2
Time-resolved UV atomic Absorption-spectroscopy.						
75 GAU/SNE	RL	300	(8.0±2.0)			2/2
k _{ref} : $O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 GAU/SNE	RN	300	3.55(14)			2	
76 DAV/SAD	RL	298	2.0			2/2	
$k_{\text{ref}}: \text{O}(^1\text{D}) + \text{CO}_2 \rightarrow \text{O} + \text{CO}_2.$							
76 DAV/SAD	EX	298	(1.45±0.03)(13)			2	
76 STR/HOW	EX	103-393	1.45(14)	0	0	2	1.1
78 DAV/SCH ³⁾	EX	300	(1.45±0.22)(14)			2	
78 DAV/SCH ³⁾	EX	103-393	1.45(14)	0	0	2	
³⁾ Quadrupled-laser photolysis.							
O + H (+ M) → OH(A²Σ⁺, v=n) (+ M)							
Oxygen atom + Hydrogen atom							
76 KOI/MOR	ES	1250-2000	1.0(9)	0	5536	3	
M = Ar. n = 0.							
76 TIC	EX	298	2.71(1)			2	
n = 1.							
76 TIC	EX	298	5.80(11)			3	
M = H. n = 0.							
76 TIC	EX	298	6.17(9)			3	
M = H ₂ . n = 0.							
76 TIC	EX	298	1.45(10)			3	
M = H. v = 1.							
82 HID/TAK	EX	1200-3200	1.2(13)	0	3493	3	
H ₂ /O ₂ mixtures in Ar diluent, heated behind reflected shock-waves. n = 0. P ₀ = (50-100 torr).							
82 KOI/MOR1	EX	1250-3450	8.32(13)	0	4177±604	3	1.48
Reaction of O and H atoms in Argon diluent. O and H atoms generated by dissociation of O ₂ and H ₂ molecules in Ar, behind incident shock-waves. P ₀ = (6-30) torr. n = 0.							
O + H₂ → OH + H							
Oxygen atom + Hydrogen molecule							
71 BRA/BEL1	EX	1200-1600	2.96(13)	0	4932±654	2	1.53
72 SCH/GET	RL	1700-2000	(4.0±1.0)			2/2	
$k_{\text{ref}}: \text{H} + \text{O}_2 \rightarrow \text{OH} + \text{O}$							
72 SCH/GET	RN	1700	4.5(12)			2	
73 GET	RN	1400-1900	3.2(14)	0	7549	2	1.25
74 NAM/TRO	EX	839-924	7.23(10)			2	
E _a not determined. Within the given T-range, k increases from 7.23x10 ¹⁰ to 1.33x10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 RAW/GAR2 k _{ref} : OH + OH → H ₂ O + O.	RL	1200-2000	2.9	0	3248	2/2	
74 RAW/GAR2	RN	1200-2000	1.6(14)	0	6808	2	
74 SCH/GET k _{ref} : O ₂ + H → O + OH	RL	1400-1900	(3.60±0.72)			2/2	
74 SCH/GET	RN	1400-1900	2.2(14)	0	6916±2406	2	1.25
75 BIR/KAS Upper-limit k. H ₂ is vibrationally excited with v' = 1.	EX	300	≤6.0(10)			2	
75 CAM/HAN2	EX	363-490	(3.1±0.5)(13)	0	4950±300	2	
75 DUB/MCK Air-afterglow.	EX	347-832	(5.30±3.01)(12)	0	4198±241	2	
75 DUB/MCK Resonance-fluorescence.	EX	347-832	(4.99±2.29)(12)	0	4330±241	2	
78 LIG 1) OH is in ground state. Upper-limit k.	EX	302	≤2.83(9)			2	
78 LIG 1) OH is either in ground state or vibrationally excited with v'' = 1.	EX	302	(6.02±5.42)(9)			2	
78 LIG 1) OH is vibrationally excited with v'' = 1.	EX	302	(6.02±3.61)(9)			2	
1) Flow-tube with tunable dye laser. H ₂ is vibrationally excited with v' = 1. P(Total) = 3 torr.							
80 BAS/KOG 2) n = 0 assumed.	EX	450-1160	1.51(13)	0	4479±201	2	1.26
80 BAS/KOG 2)	EX	450-1160	6.56(12)	0.5	4127±191	2	1.26
80 BAS/KOG 2) Extended T-range expression. Given with caution.	EX	293-1160	8.21(7)	6.4	302±332	2	100.
2) Combustion of H ₂ + O ₂ mixtures in a jet reactor. Gas-chromatography. Arrhenius preexponential factor expressed as: A(T/298) ⁿ in the expressions with n ≠ 0.							
80 LIG/MAT Flow-tube apparatus. Laser-induced Fluorescence. P = 3 torr.	EX	298	(5.5±3.0)(6)			2	
82 PAM/SKI1 Reaction of O with H ₂ behind reflected shock-waves, using H ₂ /N ₂ O/Ar mixtures. [O] _{max} = (1.7-6.6)×10 ¹³ molec.cm ⁻³ . P = (920-1224) torr.	EX	1919-2781	2.3(14)	0	6916	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err.
82 PAM/SKI2 Reaction of O with H ₂ behind reflected shock-waves, in H ₂ /O ₂ /Ar mixtures. Resonance-absorption spectroscopy. P = (1.16-2.67) atm. [O] = (5.42x10 ⁸ -3.49x10 ¹²) molec.cm ⁻³ .	EX	1000-2500	4.2(14)	0	6916	2	
O + D₂ → OD + D							
Oxygen atom + Deuterium molecule							
75 APP/APP Arrhenius preexponential factor expressed as: A(T/298) ¹ .	ES	1700-3100	1.22(13)	1.0	8254	2	2.0
82 PAM/SKI1 Reaction of O with D ₂ behind reflected shock-waves, using H ₂ /N ₂ O/Ar mixtures. [O] _{max} = (1.9-7.2)x10 ¹³ molec.cm ⁻³ . P = (920-1224) torr.	EX	2097-2481	1.6(14)	0	7169	2	
82 PAM/SKI2 Reaction of O with D ₂ behind reflected shock-waves, in D ₂ /O ₂ /Ar mixtures. Resonance-absorption spectroscopy. P = (1.16-2.67) atm. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ .	EX	1000-2500	1.9(14)	0	7169	2	
O(¹D) + H₂ → OH + H							
Oxygen atom + Hydrogen molecule							
73 HEI/HUS2	EX	300	(1.63±0.18)(14)			2	
73 HEI/HUS2 k _{ref} : O(¹ D) + N ₂ O → products.	RL	300	1.23			2/2	
75 GAU/SNE k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺)	RL	300	(4.0±1.0)			2/2	
75 GAU/SNE	RN	300	1.81(14)			2	
75 STI/PAY k _{ref} : O(¹ D) + O ₂ → O(³ P) + O ₂	RL	300	(4.23±1.80)			2/2	
75 STI/PAY	RN	300	(1.51±0.90)(14)			2	
76 DAV/SAD k _{ref} : O(¹ D) + CO ₂ → O(³ P) + CO ₂ .	RL	298	1.08			2/2	
76 DAV/SAD	RN	298	(7.83±0.30)(13)			2	
77 DAV/SCH k _{ref} : O(¹ D) + CO ₂ → O(³ P) + CO ₂ .	RL	298	9.9(-1)			2/2	
77 DAV/SCH	RN	298	(5.96±1.81)(13)			2	
78 DAV/SCH ¹⁾	EX	300	(7.83±1.17)(13)			2	
78 DAV/SCH ¹⁾	EX	204-35	5.96(13)	0	0	2	

¹⁾ Quadrupled-laser photolysis.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 PRA/FAU Photolysis of O ₂ /H ₂ mixtures diluted in He. P(O ₂) >15 torr. P(He) = 600 torr. k _{ref} = O(¹ D) + O ₂ → O(³ P) + O ₂	RL	298	(5.27±0.31)			2/2	
82 OGR/SWO Flash-photolysis of O ₂ /O ₃ /H ₂ mixtures in a vacuum system. P(Total) = 100 torr.	EX	298	(6.5±0.5)(13)			2	
O(¹D) + D₂ → OD + D							
Oxygen atom + Deuterium molecule							
73 HEI/HUS2	EX	300	(1.08±0.12)(14)			2	
76 DAV/SAD k _{ref} : O(¹ D) + CO ₂ → O(³ P) + CO ₂ .	RL	298	1.08			2/2	
76 DAV/SAD	RN	298	(7.83±0.30)(13)			2	
O + OH → O₂ + H							
Oxygen atom + Hydroxyl							
76 KRI OH is in vibrational state v=9.	EX	298	1.81(13)			2	
77 CAM/HAN k _{ref} : CO + OH → CO ₂ + H	RL	425	(2.60±0.20)(2)			2/2	
77 CAM/HAN	RN	425	(2.65±0.52)(13)			2	
77 SPE/END ¹⁾	EX	295	(5.42±1.81)(13)			2	
77 SPE/GLA ¹⁾	EX	295	(6.32±3.19)(13)			2	
¹⁾ OH is in vibrational state v=1.							
80 HOW/SMI Discharge-flow reactor. H ₂ O Flash-photolysis. Resonance-fluorescence. P(Total) = 3.75 torr.	EX	298	(2.29±0.54)(13)			2	
80 LEW/WAT ²⁾ n = 0 assumed.	EX	221-499	(1.21±0.11)(1)	0	-112±29	2	
80 LEW/WAT ²⁾ The preexponential factor expressed as: A(T/298) ^{-0.362} .	EX	221-499	1.82(13)	-0.36	0	2	1.52
²⁾ Discharge-flow-Resonance-fluorescence. [O] = (1-7)×10 ¹² molec.cm ⁻³ . [NO] ~ 1.5×10 ¹¹ molec.cm ⁻³ .							
81 HOW/SMI Discharge-flow system. OH formed by Flash-photolysis of H ₂ O. O atoms formed by reacting N with NO. Resonance-fluorescence. The preexponential factor expressed as: A(T/298) ^{-0.50} . [O] = (0.5-6.0)×10 ¹³ molec.cm ⁻³ .	EX	250-515	(2.32±0.08)(13)	-0.50	0	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + HO₂ → OH + O₂						
Oxygen atom + Hydroperoxo						
73 PEE/MAH1	ES	1600	≈5.0(13)			2
77 BUR/HAR	EX	293	(2.13±0.60)(13)			2
77 SHA	ES	250-2000	8.25(12)	0.75	0	2
The preexponential factor expressed as: A(T/298) ^{0.75} .						
78 CAM/ROG	RL	425	(3.5±1.5)(1)			2/2
k _{ref} : H + HO ₂ → products. Discharge-flow reactor. P(Total) = (0.2-0.5) kPa.						
78 PRE	EX	293	(1.5±0.5)(13)			2
Laser Magnetic Resonance Spectrometry.						
79 BUR/CLI	EX	298	(1.87±0.60)(13)			2
Conventional discharge-flow system.						
79 HAC/PRE2	EX	298	(2.0±0.6)(13)			2
Isothermal discharge-flow reactor. ESR- LMR-spectrometry. P(He) < 10 mbar.						
80 LII/SAU	EX	298	(4.21±1.20)(13)			2
Electron pulse-radiolysis. Kinetic Spec- trophotometry. P(Total) = 1200 torr.						
82 KEY2 ¹⁾	EX	229-372	(1.86±0.24)(13)	0	-200±28	2
82 KEY2 ¹⁾	EX	299	(3.67±0.24)(13)			2
¹⁾ Discharge-flow. Resonance-fluorescence. HO ₂ generated by reacting F with H ₂ O ₂ , or Cl with an excess of CH ₃ OH and O ₂ . O a- toms produced by dissociating O ₂ in a microwave-discharge. P = 1 torr. [HO ₂] = (0.7-3.3)x10 ¹² molec.cm ⁻³ . [O] ₀ = (0.4-1.9)x10 ¹¹ molec.cm ⁻³ .						
82 SRI/QIU	EX	296	(3.25±0.54)(13)			2
Discharge-flow reactor. Laser-induced- fluorescence. UV-resonance-fluorescence. HO ₂ radicals generated by reacting F with H ₂ O ₂ . F atoms generated by dissociation of CF ₄ in a microwave-discharge. H and O atoms generated by dissociation of H ₂ and O ₂ in a microwave-discharge. [H] ₀ = [O] ₀ ~ (4-5)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)x10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8x10 ¹² molec.cm ⁻³ . [NO] ~ 2x10 ¹⁴ molec.cm ⁻³ . P(He) ~ 2.5 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + H₂O → H + HO₂ (a)						
→ OH + OH (b)						
Oxygen atom + Water						
79 HAC/PRE1 k _a . Isothermal flow. Laser Magnetic Resonance-Spectrometry. M = He. k ₁ = Kk ₋₁ . P(Total) = (130-800) Pa.	DE	298	7.4(-30)			2
71 ALB/HOY k _b .	EX	753-1045	4.0(13)	0	8707±252	2
O(¹D) + H₂O → O₂ + H₂ (a)						
→ OH + OH (b)						
→ OH* + OH (c)						
Oxygen atom + Water						
80 ZEL/WAG k _a /k _b . Reaction of Oxygen atoms with Water vapor. Flash-photolysis. O(¹ D) atoms generated by photolysis of Ozone. P(O ₃) = 0.6 torr. P(H ₂ O) = (2-4) torr. P(He) = (8-11) torr.	RL	298	≤1.5(-2)			2/2
71 SCO/CVE k _b /k _{ref} . k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ (a) → NO + NO (b)	RL	296	(1.50±0.06)			2/2
72 FOR/SNE k _b /k _{ref} . k _{ref} : O(¹ D) + N ₂ → O + N ₂	RL	295	(3.5±1.5)			2/2
72 SIM/HEI2 k _b /k _{ref} . Estimated ratio. k _{ref} : O(¹ D) + CO → O(³ P) + CO	RL	300-423	3.79(-1)	0	-624	2/2
73 HEI/HUS1 k _b .	EX	300	(1.81±0.18)(14)			2
73 HEI/HUS1 k _b /k _{ref} . k _{ref} : O(¹ D) + O ₂ → products.	RL	300	4.4			2/2
73 HEI/HUS3 k _b . Time-resolved UV atomic Absorption-spectroscopy.	EX	300	(1.81±0.18)(14)			2
73 SIM/HEI2 k _b /k _{ref} . k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ (a) → NO + NO (b)	RL	373	(2.1±0.3)			2/2
75 GAU/SNE k _b /k _{ref} . k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺)	RL	300	(5.0±1.5)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 GAU/SNE k_b .	RN	300	2.23(14)			2	
76 DAV/SAD k_b/k_{ref} . $k_{ref}: O(^1D) + CO_2 \rightarrow O + CO_2$.	RL	298	1.75			2/2	
76 DAV/SAD k_b .	RN	298	(1.26±0.60)(13)			2	
76 STR/HOW k_b .	EX	253-353	1.39(14)	0	0	2	1.1
77 DAV/SCH k_b/k_{ref} . $k_{ref}: O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$.	RL	298	2.3			2/2	
77 DAV/SCH k_b .	RN	298	(1.39±0.24)(14)			2	
72 LIS/HEI k_b/k_{ref} . Ozone Photolysis. $k_{ref}: O(^1D) + O_3 \rightarrow O_2 + O_2^*$	RL	298	1.5			2/2	
78 DAV/SCH ¹⁾	EX	300	(1.26±0.19)(14)			2	
78 DAV/SCH ¹⁾	EX	253-353	1.39(14)	0	0	2	
¹⁾ k_b . Quadrupled-laser photolysis.							
79 LEE/SLA k_b . O ₂ -pulsed photolysis.	EX	300	(1.57±0.30)(14)			2	
81 GER/COM k_b . UV-Flash-photolysis Ozone in presence of H ₂ O vapor. P(H ₂ O) = (2.5-19) torr. P(O ₃) = 1.5 torr.	EX	298	(1.22±0.25)(14)			2	
81 PRA/PAU k_b/k_{ref} . Photolysis of O ₂ /H ₂ O mixtures diluted in He. P(O ₂) >15 torr. P(He) = 600 torr. $k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$.	RL	298	(6.7±0.4)			2/2	
71 PRA/VIL ²⁾ k_c/k_{ref} . $k_{ref}: O(^1D) + M \rightarrow O + M$.	RL	293	(2.0±0.5)(1)			2/2	
71 PRA/VIL ²⁾ k_c . Lower limit k.	RN	293	≥1.2(14)			2	
²⁾ Photolysis of an O ₂ + H ₂ O mixture. P(O ₂) = (30-100) Tor.							
71 PAR/CVE ³⁾ $k_{ref}: O(^1D_2) + O_2 \rightarrow$ products.	RL	298	1.07(1)			2/2	
71 PAR/CVE ³⁾ $k_{ref}: O(^1D_2) + N_2 \rightarrow$ products.	RL	298	9.64			2/2	
71 PAR/CVE ³⁾ $k_{ref}: O(^1D_2) + CO_2 \rightarrow$ products.	RL	298	2.98			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 PAR/CVE ³⁾ k _{ref} : O(¹ D ₂) + (CH ₃) ₄ C → products. ³⁾ (k _a + k _b + k _c)/k _{ref} . Photolysis of N ₂ O/ Neopentane/SF ₆ mixtures. P(Total) ~ 320 torr.	RL	298	3.76(-1)			2/2
O + H₂O₂ → OH + HO₂ (a) (predominant path) → H ₂ O + O ₂ (b)						
Oxygen atom + Hydrogen peroxide						
71 ALB/HOY k _a + k _b .	EX	370-800	2.8(13)	0	3221±302	2
74 DAV/WON k _a + k _b .	EX	283-368	(1.66±0.25)(12)	0	2125±261	2
82 ROS k _a + k _b . (Recommended expression). Conventional fast-flow system. O atoms generated by reacting N with NO in a microwave discharge. Mass-spectrometry. P[H ₂ O ₂] ₀ = (0.3-1.5)×10 ¹⁸ molec.cm ⁻³ . P = (0.9-1.7) torr.	SE	302-349	(1.66±0.25)(12)	0	2125±261	2
O(¹D) + H₂O₂ → OH + HO₂						
Oxygen atom + Hydrogen peroxide						
76 FLE/HUS	EX	300	(3.13±0.36)(14)			2
O + SO (+ M) → SO₂ (+ M)						
Oxygen atom + Sulfur monoxide						
71 MIY/TAK1 M = Ar.	EX	298	(7.40±0.73)(16)			3
79 GRI/REE M = Ar. Reflected shock-waves. k ₁ = k ₋₁ K. The preexponential factor expressed as: A(T/298) ^{-1.84} .	DE	300-3880	3.36(17)	-1.84	0	3
O + SO₂ (+ M) → O₂ + SO (+ M) (a) → SO ₃ (+ M) (b)						
Oxygen atom + Sulfur dioxide						
80 GRI/REE k _a . Thermolysis of SO ₂ diluted in N ₂ O/Ar mixtures behind reflected shock-waves.	EX	2630-3570	(4.0±0.4)(12)	0	9210	2
80 SLA/GRI k _a . Shock-heated mixtures of SO ₂ /N ₂ O mixtures behind reflected shock-waves, in presence of Ar.	EX	3320-3760	(3.8±0.5)(11)	0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 WES/DEH2 k _b . M = He. M-efficiencies relative to He are: 1.0(He), 2.4(N ₂), 9.5(SO ₂).	EX	297	(3.0±0.2)(14)			2
75 WES/DEH2 k _b . M = He.	EX	248-415	(3.9±0.9)(16)	0	1400±50	2
74 ATK/PIT3 k _b . M = N ₂ .	EX	299-392	3.32(16)	0	1007±201	3
78 ATK/PIT4 ¹⁾ k _b . M = Ar.	EX	299-440	1.12(16)	0	1009±151	3
78 ATK/PIT4 ¹⁾ k _b . M = Ar.	EX	299	(3.81±0.76)(14)			3
78 ATK/PIT4 ¹⁾ k _b . M = SO ₂ .	EX	299	(3.45±1.09)(15)			3
78 ATK/PIT4 ¹⁾ k _b . M = N ₂ .	EX	300	(4.97±0.98)(14)			3
1) Flash-photolysis. NO ₂ chemiluminescence.						
79 AST/GLA k _b . M = Ar. Incident pr reflected shock-waves. [Ar] = (0.5-4.2)×10 ¹⁹ molec.cm ⁻³ . Rate constant expressed as k[Ar]. Based on: k ₁ = Kk ₋₁ .	DE	1700-2500	1.06(13)	0	-7870	3
79 MER/LEV ²⁾ k _b /k _{ref} . k _{ref} : O + SO ₂ → O ₂ + SO ₂	RL	1685	6.6(3)			3/2
79 MER/LEV ²⁾ k _b .	ES	2250	7.4(14)			3
2) Combustion in a quartz-tube burner. M = CH ₄ , N ₂ , O ₂ , H ₂ S.						
82 SMI/TSE k _b . Reaction of SO ₂ with O in a CO/O ₂ /Ar flame. Mass-spectrometry. P = 200 torr.	EX	1435-1850	4.4(14)	0	-3163	3
O + SO ₃ (+ M) → O ₂ + SO ₂ (+ M)						
Oxygen atom + Sulfur trioxide						
71 MER/LEV k determined in H ₂ S flame.	EX	1100-1400	6.5(14)	0	5435	2
71 MER/LEV k determined in COS flame.	EX	900-1600	2.8(14)	0	6039	2
72 JAC/WIN Average of 8 experimental points.	EX	300	2.79(7)			2
72 JAC/WIN Average of 7 experimental points.	EX	413	4.22(7)			2
72 JAC/WIN Average of 6 experimental points.	EX	500	5.31(7)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 JAC/WIN A and B recalculated from the above three k's. The A-factor given in the initial abstract ($3.0 \times 10^{15} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$) should be 3.0×10^{16} .	ES	300-487	(1.40 ± 0.27)(8)	0	487±79	2
79 MER/LEV Combustion in a quartz-tube burner.	RN	1685	1.5(11)			2
82 SMI/TSE Reaction of SO ₂ with O in a CO/O ₂ /Ar flame. Mass-spectrometry. P = 200 torr.	EX	1435-1850	1.32(12)	0	3070	2
75 WES/DEH1 M = He. M-efficiencies relative to He are: 1.0(He), 1.4(N ₂), <10.0(SO ₃).	EX	298	(7.3 ± 0.2)(17)			3
75 WES/DEH1 M = He.	EX	298-507	5.0(16)	0	-785	3
O + S₂O → SO + SO						
Oxygen atom + Sulfur oxide (S ₂ O)						
74 STE/ALV	ES	298	(9.03 ± 1.20)(11)			2
O + SH → H + SO						
Oxygen atom + Mercapto						
75 CUP/GLA	EX	295	(9.64 ± 3.01)(13)			2
O + H₂S → OH + SH (a)						
→ [H ₂ SO] [‡] → HSO + H (b)						
→ [H ₂ SO] [‡] → products (c)						
Oxygen atom + Hydrogen sulfide						
76 WHY/TIM k _a . Flash-photolysis. Resonance-fluorescence. Same data given in 78 WHY/TIM.	EX	263-495	(4.36 ± 0.64)(12)	0	1661±50	2
78 SLA/BAI k _b . Fast flow-reactor. Photoionization Mass-spectrometer. A and B (not explicitly given) recalculated from the reported experimental data.	EX	281-497	(1.30 ± 0.36)(13)	0	1815±139	2
79 SIN/IRW k _a + k _b + k _c . Phase-shift. Gas-chromatography.	EX	297-502	(1.56 ± 0.83)(13)	0	2171±202	2
82 SIN/PAR ¹⁾ k _a /(k _a + k _b + k _c). Based on the reported lower-limit (0.52) and upper-limit (1.0) ratios.	RL	298	(7.6 ± 2.4)(-1)			2/2
82 SIN/PAR ¹⁾ k _b /(k _a + k _b + k _c). Upper-limit ratio.	RL	298	<2.0(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k units factor	err.
82 SIN/FAR ¹⁾ k _c /(k _a + k _b + k _c). Upper-limit ratio. Product of path (c) cannot be HSOH.	RL	298	<4.8(-1)			2/2	
¹⁾ Reaction of O with H ₂ S in a quartz cell, in N ₂ O/H ₂ /CO mixtures. O atom generated by Hg-sensi- tized decomposition of N ₂ O. Gas-chromatography. P(Total) = (368-743) torr. P(H ₂ S) = (5.5-21) torr. P(CO) = (50-200) torr.							
O + D ₂ S → OD + SD Oxygen atom + Hydrogen sulfide (D ₂ S)							
76 WHY/TIM	EX	298-450	(6.32±3.43)(12)	0	2144±156	2	
O + N (+ M) → NO (+ M) Oxygen atom + Nitrogen atom							
73 CAM/GRA ¹⁾	EX	196	(4.38±0.38)(15)			3	
73 CAM/GRA ¹⁾	EX	298	(3.34±0.36)(15)			3	
¹⁾ M = N ₂ .							
O + N ₂ (+ M) → NO + N (+ M) (a) → N ₂ O (+ M) (b) Oxygen atom + Nitrogen molecule							
73 BAC/EBE k _a .	EX	1900-2500	5.0(13)	0	37947	2	2.0
73 IVE/BAS k _a .	ES	1900-2400	1.3(14)	0	37947	2	
76 HAR/NAS k _a . Best fit to the experimental data.	EX	2270-2620	(9.1±0.4)(13)	0	38000	2	
77 BLA/SME k _a .	EX	1880-2350	7.5(13)	0	38249	2	1.2
77 MON/HAN2 k _a .	EX	2384-3850	1.84(14)	0	38374	2	1.35
79 MON/HAN k _a . Shock tube. IR-emission. CO-laser absorption.	EX	2384-3850	(1.84±0.64)(14)	0	38374	2	
71 STU/NIK1 k _b . M = N ₂ . Upper-limit k.	EX	300	<1.81(10)			3	
O(¹ D) + N ₂ (+ M) → N ₂ O (+ M) (a) → other products (b) Oxygen atom + Nitrogen molecule							
73 GAE/GLA k _a . Expressed as: k = [N ₂]1.0x10 ¹² cm ⁶ mol ⁻² s ⁻¹ .	ES	300	≈1.0(12)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PRA/PAU k_b . Photolysis of O_2/N_2 mixtures diluted in He. $k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$. P(He) = 600 torr. P(O_2) >15 torr.	RL	298	(7.21±0.79)(-1)			2/2
72 SIM/LIS k_a . M = N_2 . Upper-limit ratio. k_{ref} : $O(^1D) + M \rightarrow O + M$.	RL	298	<4.82(-2)			3/2
$O + N_3 \rightarrow NO(A^2\Sigma^+) + N_2$						
Oxygen atom + Azide						
79 PIP/KRE Na N_3 thermolysis. Conventional flow-system.	EX	461	(6.02±2.41)(12)			2
$O + NO (+ M) \rightarrow O_2 + N (+ M)$ (a)						
$\rightarrow NO_2 (+ M)$ (b)						
Oxygen atom + Nitrogen oxide (NO)						
74 HAN/FLO k_a . The preexponential factor expressed as: $A(T/298)^1$.	EX	2500-4100	7.03(11)	1.0	19446	2
77 MCC/KRU ¹⁾	EX	1750-2100	5.13(11)	1.0	19446	2 1.26
77 MCC/KRU ¹⁾ Based on a curve-fit of all previous k's. Recommended k. Same data given in 76 MCC/KRU.	RE	1750-2100	1.11(12)	1.0	20851	2
¹⁾ k_a . Flow reactor. The preexponential factor expressed as: $A(T/298)^1$.						
73 GAE/GLA k_b . M = N_2 . Limiting high-pressure k.	RN	300	8.0(12)			2
73 HAR/JOH $k_b[M]/k_{ref}$. M = N_2 . k_{ref} : $O + NO_2 \rightarrow O_2 + NO$.	RL	296	(1.8±0.1)(-1)			2/2
75 GAE/TRO k_b . M = N_2 . Limiting high-pressure k.	EX	296	(1.8±0.3)(13)			2
75 HIP/SCH k_b . M = N_2 . Limiting high-pressure k.	RN	295	(1.8±0.3)(13)			2
75 SIN/FUR k_b . M = N_2O .	EX	298-473	(6.12±0.45)(15)	0	-619±28	2
76 MIC/PAY k_b . M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 0.87(He), 0.73(Ne), 0.96(Kr), 1.64(N_2) art 217 K. 1.0(Ar), 0.95(He), 0.80(Ne), 0.99(Kr), 1.66(N_2) at 298 K. 1.0(Ar), 1.04(He), 0.89(Ne), 1.01(Kr), 1.68(N_2) at 500 K.	EX	217-500	(3.27±0.42)(15)	0	-594±35	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 MIC/PAY k_b . M = He.	EX	217-500	(3.91±0.44)(15)	0	-523±30	2	
76 MIC/PAY k_b . M = Ne.	EX	217-500	(3.38±0.40)(15)	0	-518±30	2	
76 MIC/PAY k_b . M = Kr. n = 0 assumed.	EX	217-500	(3.45±0.40)(15)	0	-574±35	2	
76 WHY/MIC1 k_b . M = N ₂ .	EX	217-500	(5.62±0.73)(15)	0	-584±35	2	
76 WHY/MIC1 k_b . M = N ₂ . The preexponential factor expressed as: A(T/298) ^{-1.82}	EX	217-500	4.33(16)	-1.82	0	2	
77 ATK/PER1 k_b . M = Ar.	EX	298-439	5.30(15)	0	-473±101	2	
77 ATK/PER1 k_b . M = Ar.	EX	298	(2.55±0.25)(16)			2	
71 ATK/CVE k_b . M = N ₂ O.	EX	298	(3.7±0.8)(16)			3	
71 STU/NIK1 k_b . M = He. M-efficiencies relative to He are: 1.0(He), 2.26(NO).	EX	300	2.41(16)			3	1.1
71 STU/NIK2 k_b .	EX	300	2.47(16)			3	
72 ATK/CVE k_b . M = N ₂ O.	EX	298-473	(2.6±0.21)(15)	0	-805±151	3	
74 ATK/PIT1 k_b . M = N ₂ O.	EX	300-392	9.6(15)	0	-453±101	3	
74 ATK/PIT2 k_b . M = N ₂ O.	EX	300	(4.30±0.43)(16)			3	
74 FUR/ATK k_b . M = N ₂ O.	EX	298	(5.78±0.08)(16)			3	
75 CAM/HAN2 k_b . M = N ₂ . M-efficiencies relative to N ₂ are: 1.0(N ₂), 0.62(Ar).	EX	285-432	(1.8±0.5)(15)	0	-900±85	3	
75 HIP/SCH k_b . M = N ₂ . Limiting low-pressure k. Reevaluation. Rate constant expressed as k/[M]. M-effi- ciencies relative to N ₂ are: 1.00(N ₂), 0.65(He), 0.86(Ne), 1.28(Ar), 1.21(CO), 1.65(CO ₂), 1.66(SF ₆), 1.43(CH ₄), 1.15(C ₂ H ₆), 1.33(cy-C ₃ H ₈), 2.13(C ₃ F ₈), 1.36(2,2-Dimethylpropane), 1.36(2,2-Dimethylbutane), 1.68(Isopropylbromide).	RN	295	(2.7±0.5)(16)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 AND k _b . M = Ar. NO Flash-photolysis. Time-resolved detection of NO ₂ chemiluminescence.	EX	298	(2.80±0.18)(16)			3
78 ATK/PIT4 ²⁾ M = SO ₂ .	EX	299	(9.43±3.27)(16)			3
78 ATK/PIT4 ²⁾ ²⁾ k _b . Flash-photolysis. NO ₂ chemiluminescence.	EX	300	(3.99±0.73)(16)			3
78 MIC/PAY1 k _b . M = N ₂ . Flash-photolysis.	EX	217-500	(5.62±0.73)(15)	0	-582±37	3
79 AND/STE k _b . M = Ar. NO vacuum-UV Flash-photolysis. Time-resolved detection of NO ₂ chemiluminescence.	EX	237-397	(4.61±0.73)(15)	0	-508±50	3
79 MIC/LEE ³⁾ k _b . M = He. n = 0 assumed.	EX	217-500	(3.92±0.44)(15)	0	-523±30	3
79 MIC/LEE ³⁾ k _b . M = He.	EX	217-500	2.60(16)	-1.63	0	3
79 MIC/LEE ³⁾ k _b . M = Ar. n = 0 assumed.	EX	217-500	(3.27±0.42)(15)	0	-594±35	3
79 MIC/LEE ³⁾ k _b . M = Ar.	EX	217-500	2.50(16)	-1.86	0	3
79 MIC/LEE ³⁾ k _b . M = N ₂ . n = 0 assumed.	EX	217-500	(5.62±0.73)(15)	0	-584±35	3
79 MIC/LEE ³⁾ k _b . M = N ₂ .	EX	217-500	4.33(16)	-1.82	0	3
³⁾ Flash-photolysis. Resonance-fluorescence. The preexponential factor expressed as: A(T/298) ⁿ in all the expressions with n ≠ 0.						
80 SUG/ISH2 ⁴⁾ k _b . M = N ₂ .	EX	298	(2.79±0.18)(16)			3
80 SUG/ISH2 ⁴⁾ k _b . M = He.	EX	298	(1.52±0.18)(16)			3
⁴⁾ Pulse-radiolysis technique. Resonance-absorption. P(Total) = (200-100) torr.						
82 FAI/SIN k _b . M _{eff} = 1.0(N ₂ O) and 31(CH ₃ OH). Modulated Phase-shift. O atoms generated by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.	EX	298	(9.79±2.71)(12)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O(^1D) + NO \rightarrow O_2 + N$							
Oxygen atom + Nitrogen oxide (NO)							
73 HEI/HUS2	EX	300	(5.12±0.60)(13)			2	
73 HEI/HUS2	RL	300	4.3(-1)			2/2	
$k_{ref}: O(^1D) + N_2O \rightarrow \text{products.}$							
$O + NO_2 (+ M) \rightarrow O_2 + NO (+ M) (a)$							
$\quad \quad \quad \rightarrow NO_3 (+ M) (b)$							
Oxygen atom + Nitrogen oxide (NO ₂)							
72 CLY/CRU	EX	298	(3.67±0.36)(12)			2	
$k_a.$							
72 GER/DEM	EX	298	(4.0±1.0)(12)			2	
$k_a.$							
73 DAV/HER	EX	230-339	(5.49±0.27)(12)	0	0	2	
$k_a.$							
73 HAR/JOH	RN	296	5.54(12)			2	
$k_a.$							
73 SLA/WOO ¹⁾	EX	240	6.32(12)			2	1.15
73 SLA/WOO ¹⁾	EX	296	5.60(12)			2	1.15
¹⁾ $k_a.$							
74 BEM/CLY ²⁾	EX	298	(5.72±0.66)(12)			2	
74 BEM/CLY ²⁾	EX	298-1055	5.43(12)	-0.52	0	2	1.37
The preexponential factor expressed as:							
$A(T/298)^{-0.52}.$							
²⁾ $k_a.$							
74 STE/ALV	RL	298	(6.0±0.5)			2	
$k_a. \quad k_{ref}: O + S_2O \rightarrow SO + SO.$							
75 WU/NIK	EX	298	5.72(12)			2	
$k_a. \quad NO_2$ Photolysis.							
73 GAE/GLA ³⁾	RN	300	6.0(12)			2	
75 GAE/TRO ³⁾	EX	296	(1.3±0.2)(13)			2	
³⁾ $k_b. \quad M = N_2. \quad \text{Limiting high-pressure } k.$							
73 HAR/JOH	RL	296	(2.2±0.1)(-1)			2/2	
$k_b[M]/k_{ref}. \quad M = N_2. \quad k_{ref}: O + NO_2 \rightarrow O_2 + NO.$							
75 HIP/SCH	RN	295	(1.3±0.2)(13)			2	
$k_b. \quad M = N_2. \quad \text{Limiting high-pressure } k.$							
Reevaluation.							
73 HAR/JOH	RN	296	2.97(16)			3	
$k_b.$							
73 HUI ⁴⁾	EX	263	(1.45±0.44)(17)			3	
73 HUI ⁴⁾	EX	298	(7.62±2.18)(16)			3	
⁴⁾ $k_b. \quad M = Ar.$							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A k err. units factor
75 HIP/SCH M = N ₂ . Limiting low-pressure k. Reevaluation. k expressed as k/[M]. M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.94(He), 1.30(Ne), 1.38(Ar), 1.97(CO), 2.63(CO ₂), 3.60(SF ₆), 2.59(CH ₄), 2.67(C ₂ H ₆), 2.26(C ₃ H ₈), 3.15(cy-C ₃ H ₈), 4.36(CF ₄), 4.27(C ₂ F ₆), 7.11(C ₃ F ₈), 3.72(2,2-Dimethylpropane), 3.89(2,2-Dimethylbutane), 2.83(Isopropylbromide), 5.95(2,2,3-Trimethylbutane).	RN	295	(2.9±0.4)(16)			3
75 WU/NIK k _b . M = Ar. NO ₂ Photolysis.	EX	298	4.50(16)			3
O(¹D) + NO₂ → O₂ + NO						
Oxygen atom + Nitrogen oxide (NO ₂)						
73 HEI/HUS2	EX	300	(1.39±0.12)(14)			2
73 HEI/HUS2 k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ (a) → NO + NO (b)	RL	300	1.05			2
75 GAU/SNE k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺) Estimated ratio.	RL	300	~4.0			2/2
75 GAU/SNE	RN	300	1.81(14)			2
O + NO₃ → O₂ + NO₂						
Oxygen atom + Nitrogen oxide (NO ₃)						
75 GRA	RN	298-329	(6.02±1.2)(12)	0	0	2
78 GRA/JOH Modulated photolysis technique.	EX	298	(6.02±0.24)(12)			2
O + N₂O → O₂ + N₂ (a) → NO + NO (b)						
Oxygen atom + Nitrogen oxide (N ₂ O)						
72 BOR/SKA k _a /k _b . Reflected shock waves. 20% N ₂ O + 80% Ar.	RL	1000-2000	(8.0±3.0)(-1)	0	0	2/2
72 SOL k _a .	SE	1000-3000	4.5(13)	0	12128	2
75 DOV/NIP k _a + k _b .	EX	2160-3400	5.25(13)	0	12557±1122	2 1.58
76 DEA k _a . Data-fit to a proposed mechanism. Same data given in 75 BAB/DEA.	ES	1950-3075	1.15(13)	0	12630	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 MON/HAN1 $k_a = k_b$. Best data-fit.	ES	1815-3365	6.23(13)	0	12350	2	1.65
77 BAL/VAN k_a . Supersonic molecular beam. Mass-spectrometer. P = 40 torr. Based on the k for the reaction: $O + N_2O \rightarrow NO + NO$.	EX	1900	(5.9±1.8)(11)			2	
77 DEA/STE1 k_a . M = Ar. Shock-waves. $N_2O/CO/Ar$ mixtures at a Total concentration of $(2.5-7.7) \times 10^{18}$ molec. cm^{-3} .	EX	2100-3200	4.64(13)	0	14073	2	
80 SUL/KLI k_a . Thermolysis of N_2O behind shock-waves, diluted in Ar. P = (1300-3500) torr.	EX	1685-2000	(4.43±3.97)(13)	0	6215±1198	2	
80 ZAS/LOS k_a . Thermolysis of (0.5-2.5)% N_2O in Ar, He, N_2 , or CO, behind shwaves. [M] = $(0.6-6.0) \times 10^{19}$ molec. cm^{-3} .	EX	1700-2500	2.6(13)	0	11072	2	
71 LIP ¹⁾	RL	1400-2000	(5.1±1.6)(-1)				2/2
73 LIP/MIL ¹⁾	RL	1300-1950	5.0(-1)				2/2
73 MIL/MAT ¹⁾ Average rate-ratio.	RL	1169-1650	(3.17±2.70)(-1)				2/2
76 MIL ¹⁾	RL	1216-1655	(2.52±1.35)(-1)				2/2
76 MIL ¹⁾ Average rate-ratio.	RL	1370-1655	2.75(-5)				2/2 2.45
¹⁾ k_b/k_a .							
72 SOL k_b .	SE	1000-3000	4.5(13)	0	12128	2	
76 DEA k_b . fit to a proposed mechanism. Same data given in 75 BAB/DEA.	ES	1950-3075	1.15(13)	0	12630	2	
77 BAL/VAN k_b . Supersonic molecular beam. Mass-spectrometer. P = 40 torr.	EX	1800-2000	(5.4±1.6)(14)	0	16105	2	
77 DEA/STE1 k_b . M = Ar. Shoch waves.. $N_2O/CO/Ar$ mixtures. Conc.(Total) = $(2.5-7.7) \times 10^{18}$ molec. cm^{-3} .	EX	2100-3200	4.64(13)	0	14073	2	
80 SUL/KLI k_b . M = Ar. Thermolysis of N_2O behind reflected shock-waves. P = (1300-3500) torr.	EX	1685-2000	(4.07±3.26)(13)	0	6215±1198	2	
80 ZAS/LOS k_b . Thermolysis of (0.5-2.5)% N_2O in Ar, He, N_2 , or CO behind shock-waves. [M] = $(0.6-6.0) \times 10^{19}$ molec. cm^{-3} .	EX	1700-2500	1.4(14)	0	15098	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O(^1D) + N_2O \rightarrow O_2 + N_2$ (a)						
$\rightarrow NO + NO$ (b)						
$\rightarrow N + NO_2$ (c)						
Oxygen atom + Nitrogen oxide (N_2O)						
71 GOL/GRE ¹⁾ At 228.8 nm.	RL	298	(3.3±0.3)(-1)			2/2
71 GOL/GRE ¹⁾ At 253.7 nm.	RL	298	(3.7±0.3)(-1)			2/2
¹⁾ $k_a/(k_a + k_b)$.						
71 SCO/PRE k_a/k_b . Photolysis of NO_2 and N_2O mixtures.	RL	298	(1.01±0.06)			2/2
72 GRE k_a/k_b . For completely thermalized $O(^1D)$, $k_a/k_b = 0.85±0.05$.	RL	298	(5.9±0.1)(-1)			2/2
72 SIM/GRE k_a/k_b . Rate ratio valid for $O(^1D)$ atoms with translational energy in excess of 10 kcal/mole.	RL	298	(6.5±0.7)(-1)			2/2
72 SIM/GRE k_a/k_b . Rate ratio valid for $O(^1D)$ atoms with no excess thermal energy.	RL	300	(9.0±1.0)(-1)			2/2
73 GHO/ELL k_a/k_b .	RL	298	(7.0±0.2)(-1)			2/2
74 WIE/PAR k_a/k_b .	RL	298	(1.0±0.17)			2/2
79 DAV/HOW ²⁾ k_a/k_b . UV-photolysis of pure N_2O .	RL	300	(6.80±0.18)(-1)			2/2
79 DAV/HOW ²⁾ k_a/k_b . UV-photolysis of N_2O + He mixtures.	RL	300	8.0(-1)			2/2
79 DAV/HOW ²⁾ ²⁾ Chemical-ionization mass spectrometry. ³⁾ $k_a/k_b = (0.72±0.11) + (21.6±7.0/T)$. Best data-fit.	RL	170-434	³⁾	³⁾	³⁾	2/2
79 MAR/BAH $k_a/(k_a + k_b + k_c)$. N_2O photolysis in excess He. Gas-chromatography.	RL	298	(6.17±0.15)(-1)			2/2
79 VOL/FEL ⁴⁾ k_a/k_b . Photolysis of pure N_2O . $P(N_2O) = (39-120)$ torr.	RL	290	(7.34±1.13)(-1)			2/2
79 VOL/FEL ⁴⁾ k_a/k_b . Photolysis of N_2O in He. $P(He) = (622-730)$ torr. $P(N_2O) = (29-97)$ torr.	RL	290	(9.19±1.00)(-1)			2/2
⁴⁾ Gas chromatography.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PRA/PAU k_a/k_{ref} . Photolysis of O_2/N_2O mixtures diluted in He. $k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$. P(He) = 600 torr. P(O_2) >15 torr.	RL	298	(4.6±0.3)			2/2
72 LIS/HEI ⁵⁾ At 228.8 nm.	RL	298	2.5(-1)			2/2
72 LIS/HEI ⁵⁾ At 253.7 nm. Approximate ratio.	RL	298	~4.0(-1)			2/2
72 LIS/HEI ⁵⁾ At 280 nm.	RL	298	6.7(-1)			2/2
⁵⁾ ($k_a + k_b$)/ k_{ref} . O_3 photolysis. $k_{ref}: O(^1D) + O_3 \rightarrow O_2 + O_2$						
72 LOU/CVE ⁶⁾ $k_{ref}: O(^1D) + CO_2 \rightarrow O + CO_2$	RL	298	(1.25±0.14)			2/2
72 PAR/SYM ⁶⁾ $k_{ref}: O(^1D) + (CH_3)_4C \rightarrow$ products.	RL	298	(1.45±0.10)(-1)			2/2
73 GHO/ELL ⁶⁾ $k_{ref}: O(^1D) + O_2 \rightarrow O + O_2$.	RL	298	(3.23±0.10)			2/2
⁶⁾ ($k_a + k_b$)/ k_{ref} .						
73 GHO/ELL $k_a + k_b$.	RN	298	1.2(14)			2
73 HEI/HUS2 $k_a + k_b$.	EX	300	(1.32±0.12)(14)			2
75 GAU/SNE ($k_a + k_b$)/ k_{ref} . $k_{ref}: O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$	RL	300	(3.3±0.5)			2/2
75 GAU/SNE $k_a + k_b$.	RN	300	1.45(14)			2
76 DAV/SAD ⁷⁾ ($k_a + k_b$)/ k_{ref} .	RL	298	1.25			2/2
76 DAV/SAD ⁷⁾ $k_a + k_b$.	RN	298	(8.43±0.60)(13)			2
77 DAV/SCH ⁷⁾ ($k_a + k_b$)/ k_{ref} .	RL	298	1.1			2/2
77 DAV/SCH ⁷⁾ $k_a + k_b$.	RN	298	(6.63±1.20)(13)			2
⁷⁾ $k_{ref}: O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$.						
78 DAV/SCH ⁸⁾ $k_a + k_b$.	EX	300	(8.43±1.26)(13)			2
78 DAV/SCH ⁸⁾ $k_a + k_b$.	EX	204-359	6.63(13)	0	0	2
⁸⁾ Quadrupled-laser photolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 LAM/HAS ⁷) (k _a + k _b)/k _{ref} .	RL	177	(2.9±0.4)				2/2
81 LAM/HAS ⁷) (k _a + k _b)/k _{ref} .	RL	296	(4.0±0.4)				2/2
81 LAM/HAS ⁷) k _b /k _{ref} .	RL	177-296	(6.2±0.9)(-1)				2/2
⁷) N ₂ O/N ₂ /He photolysis. P(Total) = (100-600) torr. k _{ref} : O(¹ D) + N ₂ → O(³ P) + N ₂ .							
71 SCO/PRE k _c /k _a . NO ₂ /N ₂ O photolysis. Upper-limit ratio.	RL	298	<5.0(-3)				2/2
O(¹S) + N₂O → products							
Oxygen atom + Nitrogen oxide (N ₂ O)							
76 SLA/BLA2	EX	200-368	(2.29±0.60)(13)	0	423±75		2
O + N₂O₅ → products							
Oxygen atom + Nitrogen oxide (N ₂ O ₅)							
75 GRA Upper-limit k.	RN	298	≤1.2(10)				2
78 GRA/JOH Modulated photolysis. Upper limit k.	EX	298	≤1.20(10)				2
78 KAI/JAP1 Discharge-flow. Upper-limit k. P(N ₂) = 4.5 torr.	EX	223-300	≤1.81(8)				2
O + NS → SO + N							
Oxygen atom + Nitrogen sulfide (NS)							
72 LIT/DAL	ES	300	~1.2(13)				2 2.0
O + NH₂ → OH + NH (a) → H + HNO (b)							
Oxygen atom + Amidogen							
73 GEH/HOY k _a + k _b .	EX	298	2.1(12)				2
O + NH₃ → OH + NH₂							
Oxygen atom + Ammonia							
74 DOV/NIP Upper-limit k.	EX	1620-1920	≤1.0(13)	0	3322		2
74 KIR/MER Flow reactor. Ultrasonic molecular beam.	EX	300-450	(4.9±1.5)(12)	0	3091±108		2
80 LAL/VER O ₂ photolysis in Ar. Resonance-fluorescence.	EX	298	(3.01±0.90)(9)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O(¹D) + NH₃ → OH + NH₂						
Oxygen atom + Ammonia						
76 DAV/SAD	EX	298	(2.04±0.18)(14)			2
76 FLE/HUS	EX	300	(3.79±0.42)(14)			2
77 DAV/SCH	RL	298	2.5			2/2
k _{ref} : CO ₂ + O(¹ D) → CO ₂ + O(³ P).						
77 DAV/SCH	RN	298	(1.51±0.30)(14)			2
78 DAV/SCH ¹⁾	EX	300	(2.05±0.31)(14)			2
78 DAV/SCH ¹⁾	EX	204-354	1.51(14)	0	0	2
T-independent k.						
¹⁾ Quadrupled-laser photolysis.						
O + HNO → OH + NO						
Oxygen atom + Nitrosyl hydride						
75 CAM/HAN2	RN	425	≥1.13(2)			2/2
k _{ref} : H + HNO → H ₂ + NO. Lower-limit ratio.						
O + HONO → products						
Oxygen atom + Nitrous acid						
78 KAI/JAP2	EX	300-355	≤6.02(8)	0	0	2
Discharge-flow reactor. Upper-limit k.						
O + HONO₂ → OH + NO₃						
Oxygen atom + Nitric acid						
72 MOR/SMI	EX	300	<7.82(9)			2
Upper-limit k.						
74 CHA/WAY	EX	300	≤1.81(7)			2
Upper-limit k.						
O + HO₂NO₂ → products						
Oxygen atom + Peroxynitric acid						
81 CHA/TRE	EX	228-297	(4.22±7.36)(13)	0	3369±489	2
Low-pressure stirred-flow. Discharge-flow. Modulated molecular-beam Mass-spectrometer. P ~2 torr.						
O(¹D) + CO → CO₂						
Oxygen atom + Carbon monoxide						
73 HEI/HUS1 ¹⁾	EX	300	(4.40±0.42)(13)			2
73 HEI/HUS1 ¹⁾	RL	300	1.05			2/2
k _{ref} : O(¹ D) + O ₂ → products.						
¹⁾ Time-resolved UV atomic Absorption-spectroscopy. Same data given in 73 HEI/HUS3.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PRA/PAU Photolysis of O ₂ /CO mixtures diluted in He. P(He) = 600 torr. k _{ref} = O(¹ D) + O ₂ → O(³ P) + O ₂	RL	298	(9.0±1.3)(-1)			2/2
O + CO (+ M) → CO ₂ (+ M) (a) → CO ₂ (³ B ₂) (+ M) (b)						
Oxygen atom + Carbon monoxide						
72 DEM k _a . M = CO ₂ . k increasing from 9.77x10 ⁷ to 3.5x10 ⁸ cm ³ mol ⁻¹ s ⁻¹ between 0.74 and 42 atm. Hippler and Troe's expression used.	EX	298	9.77(7)			2
72 DEM k _a . M = CO ₂ . k increasing from 5.24x10 ⁷ to 2.75x10 ⁸ cm ³ mol ⁻¹ s ⁻¹ between 0.74 and 42 atm. Sauer's expression used.	EX	298	5.24(7)			2
72 SIM/HEI1 k _a . M = N ₂ O. Limiting high-pressure k.	EX	298-472	1.6(10)	0	1459	2
73 GAE/GLA k _a . M = CO. Limiting high-pressure k.	RN	300	≤3.0(8)			2
77 DEA/STE1 k _a . M = Ar. Shock/waves. N ₂ O/CO/Ar mixtures.	EX	2100-3200	(5.80±1.09)(13)	0	0	2
71 DON/HUS ¹) k _a . M = Ar.	EX	300	(5.08±2.54)(12)			3
71 DON/HUS ¹) k _a . M = He.	EX	300	(5.08±2.54)(12)			3
¹) Kinetic Absorption-spectroscopy.						
71 MIY/TAK1 k _a . M = Ar.	EX	298	(2.11±0.61)(16)			3
71 STU/NIK1 k _a . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.77(He), 1.45(CO).	EX	300	7.98(11)			3 1.25
72 BAL/JAC k _a . M = Ar.	ES	300-3500	3.0(14)	0	1510	3
72 SIM/HEI1 k _a . M = N ₂ O. Limiting low-pressure k.	EX	298-472	5.9(15)	0	2063	3
72 SLA/WOO k _a . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00((N ₂), 1.70(CO), 2.70(CO ₂).	EX	296	(8.34±1.45)(11)			3
72 SLA/WOO k _a . M = CO.	EX	250-370	2.36(15)	0	2184±277	3
72 ZAB/HAR k _a . Upper-limit k.	EX	1400-1500	≤2.0(14)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A units	k _{err.} factor
73 INN k _a . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.46(CO), 0.55(CO ₂).	EX	296	(3.56±0.73)(12)			3	
74 HAR/VAS k _a . M = Ar. Upper-limit k.	EX	1500	<2.0(14)			3	
74 INN k _a . M = CO ₂ .	EX	257-277	8.02(14)	0	1782±408	3	
74 KON k _a . M = O ₂ . Reevaluation.	SE	400-500	2.35(12)	0	-1862	3	
74 WAG/ZAB k _a . M = Ar. Limiting low-pressure k. The preexponential factor expressed as: A(T/298) ⁻¹⁵ .	RN	298-4000	1.96(15)	-1.5	2516	3	
76 WEI k _a . M = Ar(89%) + CO(4%) + O ₂ (3%) + NO ₂ (3%). The preexponential factor expressed as: A(T/298) ⁻¹ .	EX	2500-2900	1.01(16)	-1.0	2013	3	
78 HAR/GAR k _a . M = Ar. Reflected shock-waves. Best fit of experimental data. P(Total) = (2-4) atm.	EX	1300-2200	2.79(13)	0	-2285	3	
80 SUG/ISH1 ²⁾ k _a . M = He.	EX	296	(3.63±0.73)(12)			3	
80 SUG/ISH1 ²⁾ k _a . M = CO. ²⁾ Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(1.09±0.73)(13)			3	
80 TOB/ULL k _p . M = CO ₂ . Vacuum system. P <1.0x10 ⁻⁵ torr.	EX	348-433	1.26(9)	0	805±755	2	40.0
O + CO ₂ (+ M) → O ₂ + CO (+ M) (a)							
→ CO ₃ (+ M) (b)							
Oxygen atom + Carbon dioxide							
74 BAB/DEA k _a .	EX	3015-4675	4.78(12)	0	18168±1459	2	1.58
71 STU/NIK1 k _p . M = CO. Upper-limit k.	EX	300	≤3.27(12)			3	
80 SUG/ISH1 k _p . M = He. Pulse-radiolysis. Resonance-absorption. P = (50-950) torr. Upper-limit k.	EX	296	<1.45(12)			3	
O(¹ D) + CO ₂ → O ₂ + CO							
Oxygen atom + Carbon dioxide							
73 HEI/HUS1	EX	300	(1.26±0.12)(14)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 HEI/HUS1 k _{ref} : O ₂ + O(¹ D) → products.	RL	300	3.1				2/2
75 GAU/SNE k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺).	RL	300	(2.7±0.5)				2/2
75 GAU/SNE	RN	300	1.20(14)				2
81 FRA/PAU Photolysis of O ₂ /CO ₂ mixtures diluted in He. P(He) = 600 torr. k _{ref} = O(¹ D) + O ₂ → O(³ P) + O ₂ .	RL	298	(2.82±0.20)				2/2
O + CH → products							
Oxygen atom + Methylidyne							
81 MES/FIL CH produced by IR multiple photon dissociation of CH ₃ OH in Ar. Same data given in 80 MES/CAR. P(CH ₃ OH) = 1.3 mtorr. P(Ar) = (5-15) torr.	EX	298	(5.72±0.84)(13)				2
O + CH₂ → CO + H + H (a) → CHO + H (b)							
Oxygen atom + Methylene							
73 JON/BAY1 k _a /k _{ref} . k _{ref} : CH≡CH + CH ₂ → products.	RL	298	(3.1±0.2)				2/2
79 VIN/DEB2 k _a . Oxidation of Acetylene in a fast-flow reactor. P(Total) = 2.2 torr.	EX	295	(7.83±1.81)(13)				2
82 GRE/HOM1 k _a . Reaction of the CH≡CH/O/H system diluted with He/N ₂ in a discharge-reactor. Resonance-fluorescence. O atoms generated by reacting N with O. H atoms produced by a discharge of the mixture H ₂ /He. Best fit to experiental data. P = 2 torr.	EX	298	(5.0±1.0)(13)				2
81 TSU/HAS k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures in Ar behind reflected shock-waves.	ES	1200-1800	3.02(13)	0	0		2
O + CH₃ → H + HCHO							
Oxygen atom + Methyl							
72 NIK/MOR2	EX	300	5.42(13)				2
73 MOR/NIK1 Unreported T assumed to be 298K. Lower-limit k.	EX	298	>1.81(13)				2
73 PEE/MAH1 k _{ref} : OH + CH ₄ → H ₂ O + CH ₃	RL	1100-1900	4.4	0	-2013		2/2
73 PEE/MAH1	RN	1100-1900	1.3(14)	0	1007		2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 WAS/BAY	EX	297	(7.4±0.15)(13)			2
74 SLA/PRU	EX	300	(1.11±0.17)(14)			2
75 BIO/LAZ	EX	1550-1725	1.05(14)	0	0	2
75 BOW1 Best data-fit.	ES	1900-2400	1.0(14)	0	0	2
76 WAS/BAY	EX	259-341	(6.02±1.20)(13)	0	0	2
76 TSU Computer calculation.	DE	1500-2000	6.03(13)	0	0	2
71 CLA/IZO2 Shock-waves. Time-of-flight Mass-spectrometry. Total conc. = 9×10^{13} molec.cm ⁻³ .	ES	1350	2.53(13)			2
71 DEA/KIS Shock-waves. Best-fit to experimental data. Total conc. = 5×10^{17} molec.cm ⁻³ .	DE	1750-2575	6.02(13)	0	0	2
72 MOR/NIK Discharge-flow. Time-of-flight Mass-spectrometry. Lower-limit k.	EX	298	>1.81(13)			2
80 BHA/FRA Shock-tube. Atomic Resonance-Absorption.	EX	1700-2300	(8.5±1.0)(13)	0	0	2
80 WAS Generation of CH ₃ by reaction of O with Ethene in a fast-flow reactor. Photoionization Mass-spectrometer. P(Total) = (1.9-3.7) torr. Comparable data in 79 WAS1, 79 WAS2 and 79 WAS3.	EX	298	(8.31±2.77)(13)			2
82 PLU/RVA2 Reaction of CH ₃ with O in a flow-reactor, in He. CH ₃ generated by reacting F with CH ₄ . O and F atoms generated by dissociation of O ₂ and CF ₄ in a microwave discharge. Mass-spectrometry. [He] = (6.3-13.1) × 10 ¹⁶ molec.cm ⁻³ . [O] = (0.6-5.1) × 10 ¹² molec.cm ⁻³ . [CH ₄] = (5-10) × 10 ¹² molec.cm ⁻³ . [CF ₄] = (3-8) × 10 ¹¹ molec.cm ⁻³ .	EX	295	(6.87±1.75)(13)			2
$O + CH_4 \rightarrow OH + CH_3$ (a) $\rightarrow H_2O + CH_2$ (b)						
Oxygen atom + Methane						
71 AVR/KOL1 k _a .	EX	373-583	(4.22±2.11)(13)	0	4630±352	2
71 DEA/KIS k _a . Shock-waves. Best-fit to experimental data. Total conc. = 5×10^{17} molec.cm ⁻³ .	DE	1750-2575	1.57(14)	0	4001	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 BRA/BRO k_a .	EX	1300-2000	1.9(14)	0	5900	2
77 ROT/JUS k_a .	EX	1500-2250	4.09(14)	0	7030	2
78 SHA k_a . The preexponential factor expressed as: $A(T/298)^2$.	DE	300-2500	4.55(11)	2.0	3240	2
79 FEL/FON k_a . Flash-photolysis. Resonance-fluorescence. High-temperature photolysis. The preexponential factor expressed as: $A(T/298)^{2.075}$. The reported k's are represented reasonably well by the above rate expression of Roth and Just, but are somewhat larger at higher T's.	EX	525-1250	1.59(12)	2.075	3840	2
80 FEL/FON k_a . High-T photochemistry reactor. Resonance-fluorescence. $P(N_2) = 25$ torr.	EX	1140	(5.60±0.48)(11)			2
80 KLE/TAN k_a . Flash-photolysis. Discharge-flow. Resonance-fluorescence. $P(Ar) = (100-200)$ torr.	EX	474-1156	(1.29±0.18)(14)	0	5472±97	2
80 ROT ¹)	EX	1500-2200	4.10(14)	0	7030	2
80 ROT ¹) Modified Arrhenius expression over extended T-range by combining the k's of several authors. The preexponential factor expressed as: $A(T/298)^{2.075}$.	EX	300-2200	1.59(12)	2.075	3840	2
¹) k_a . Thermolysis of N_2O behind shock-waves. Atomic Resonance-Absorption Spectrophotometry. Same data published in 79 ROT/JUS1.						
81 KLE/TAN ²)	EX	474-1156	(1.20±0.20)(14)	0	5435±112	2
81 KLE/TAN ²) Arrhenius expression extended over the upper T-range, obtained by combining the present data with the results of two previous shock tube studies. The preexponential factor expressed as: $A(T/298)^{0.5}$.	EX	475-2250	(5.45±0.34)(13)	0.5	5179±54	2
²) k_a . M = Ar. Resonance-fluorescence combined with either Flash-photolysis at a total P of (100-200) torr., or Discharge-flow at a total P of (1.1-2.9) torr.						
71 AVR/KOL1 k_b .	EX	373-583	(3.31±1.63)(12)	0	3372±352	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O(^1D) + CH_4 \rightarrow OH + CH_3$ (a) (Main channel)						
$\rightarrow H_2 + HCHO$ (b)						
Oxygen atom + Methane						
72 GRE	RL	298	(2.28±0.20)			2/2
k_a/k_{ref} . $k_{ref}: O(^1D) + N_2O \rightarrow O_2 + N_2$ (m)						
$\rightarrow NO + NO$ (n)						
For completely thermalized $O(^1D)$,						
$k_a/k_{ref} = 1.35 \pm 0.3$						
72 GRE/HEI	RL	298	(2.28±0.20)			2/2
k_a/k_{ref} . $k_{ref}: O(^1D) + N_2O \rightarrow O_2 + N_2$ (m)						
$\rightarrow NO + NO$ (n)						
With added He, $k_a/k_{ref} = (1.35 \pm 0.3)$						
73 HEI/HUS2	EX	300	(1.87±0.24)(14)			2
$k_a + k_b$.						
73 HEI/HUS2	RL	300	1.41			2/2
$(k_a + k_b)/k_{ref}$. $k_{ref}: O(^1D) + N_2O \rightarrow O_2 + N_2$ (m)						
$\rightarrow NO + NO$ (n)						
75 GAU/SNE	RL	300	(5.1±1.0)			2/2
$(k_a + k_b)/k_{ref}$. $k_{ref}: O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$						
75 GAU/SNE	RN	300	2.29(14)			2
$k_a + k_b$.						
76 DAV/SAD	RL	298	1.08			2/2
$(k_a + k_b)/k_{ref}$.						
$k_{ref}: O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$.						
76 DAV/SAD	RN	298	(7.83±1.81)(13)			2
$k_a + k_b$.						
76 JAY/SIM	RL	298	(1.1±0.2)(-1)			2/2
$k_b/(k_a + k_b)$.						
77 DAV/SCH	RL	298	1.4			2/2
$(k_a + k_b)/k_{ref}$.						
$k_{ref}: O(^1D) + CO_2 \rightarrow O(^3P) + CO_2$.						
77 DAV/SCH	RN	298	(8.43±2.41)(13)			2
$k_a + k_b$.						
78 DAV/SCH ¹⁾	EX	300	(7.83±1.17)(13)			2
78 DAV/SCH ¹⁾	EX	198-357	8.43(13)	0	0	2
T-independent k.						
¹⁾ k_a . Quadrupled-laser photolysis.						
81 PRA/PAU	RL	298	(6.85±0.13)			2/2
k_a/k_{ref} .						
Photolysis of O_2/CH_4 mixtures diluted in He.						
$k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$						
P(O_2) >15 torr. P(He) = 600 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
O + CHO → OH + CO (a)						
→ H + CO₂ (b)						
Oxygen atom + Methyl, oxo-						
73 MAC/THR $k_a/(k_a + k_b)$.	RL	300	5.4(-1)			2/2
76 KRI k_a . OH is in vibrational state $v = 9$.	EX	298	3.61(12)			2
72 WES/DEH3 k_b/k_a .	RL	298	(7.3±1.5)(-1)			2/2
73 MAC/THR $k_b/(k_a + k_b)$.	RL	300	4.6(-1)			2/2
74 WAS/MAR $k_a + k_b$. Ethylene used as source of CHO.	EX	297	(1.26±0.24)(14)			2
76 MAR $k_a + k_b$. Formaldehyde used as source of CHO.	EX	297	(1.33±0.24)(14)			2
O + HCHO → OH + CHO (a)						
→ OH + CO + H (b)						
→ H + H + CO₂ (c)						
→ products (d)						
Oxygen atom + Formaldehyde						
73 MAC/THR k_a .	EX	300	(9.0±1.0)(10)			2
79 KLE k_a . Flash-photolysis. Resonance-fluorescence. Mass-spectrometry.	EX	250-500	(1.67±0.19)(13)	0	1525±40	2
80 KLE/SKO k_a . Discharge-flow. Resonance-Fluorescence. k obtained by combining the present data with the data from reference 79 KLE (see above.)	EX	250-750	(1.77±0.16)(16)	0	1543±34	2
71 DEA/KIS k_b . Shock-waves. Best-fit to experimental data. Total conc. = 5×10^{17} molec.cm ⁻³ .	DE	1750-2575	6.02(13)	0	0	2
71 IZO/KIS k_b . Shock waves. Best-fit to experimental data. Total conc.: 5×10^{17} molec.cm ⁻³ .	DE	1400-2200	6.02(13)	0	0	2
81 MOR/HEI $k_c/(k_a + k_c)$. Photolysis NO ₂ in presence of CHO and O ₂ , at 360 nm. Upper-limit ratio. P(Total) = 52 torr.	RL	296	≤(1.6±0.2)(-1)			2/2
74 CAD/WIC k_d . Unspecified T-range near 300K.	EX	~300	3.7(12)	0	1208	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 CAD/WIC k_d .	EX	300	6.6(10)			2
79 CHA/BAR k_d . Discharge-flow system. Mas-spectrometry.	EX	296-437	(2.29±0.48)(13)	0	1583±73	2
O + CH₃OH → OH + CH₂OH (a) → OH + CH₃O (b)						
Oxygen atom + Methanol						
71 AVR/KOL2 k_a .	EX	343-413	3.01(11)	0	1409±352	2
75 BAS/KOG k_a . Reaction of O with CH ₃ OH vapor in a cylindrical reactor. O generated by decomposition of an O ₂ /He mixture in a high-frequency discharge. ESR-spectroscopy. Gas-chromatography.	EX	300-830	(4.28±0.07)(12)	0	1022±67	2
76 OWE/ROS k_a . Initial step of a proposed mechanism. Flow-reactor.	EX	301-451	1.45(9)	0	1540±144	2 1.07
81 GRO/JUS k_a . Conventional fast-flow reactor. Time-of-flight Mass-spectrometry.	EX	300-1006	(3.43±1.14)(14)	0	2750±150	2
81 KEI/TAN k_a . Discharge-flow. Flash-photolysis, or Resonance-fluorescence. P(Total) = (2.7-4.4) torr.	EX	298-998	(1.63±0.30)(13)	0	2531±81	2
82 FAI/SIN k_a . Major path. Modulated Phase-shift. O atoms generated by Hg-photosensitized decomposition of N ₂ O. Gas-chromarography.	EX	297-544	(9.79±2.71)(12)	0	2267±111	2
80 LAL/VER $k_a + k_b$. Pulsed photolysis of an O ₂ /Ar mixture. Resonance-fluorescence. P = 1 torr.	EX	298	(3.61±0.60)(7)			2
71 AVR/KOL2 k_b .	EX	343-413	6.02(12)	0	3322±352	2
72 LEF/MEA k_b .	EX	273-438	(1.70±0.66)(12)	0	1147±101	2
O(¹D) + CH₃OH → products						
Oxygen atom + Methanol						
75 OSI/SIM k_{ref} : O(¹ D) + N ₂ O → NO + NO (a) → O ₂ + N ₂ (b) ($k_{ref} = k_a + k_b$)	RL	298-345	(5.5±2.0)	0	0	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CS → CO(v=n) + S						
Oxygen atom + Carbon monosulfide						
71 HAN/SMI v≤13.	ES	298	8.43(12)			2
72 HAN/RID k _{ref} : O + CS → CO(v=13) + S. Ratio increasing from 0.1 to 0.9 between between v=7 and v=12, then decreasing to 0.3 from v = 14 to v = 15. Unreported T assumed to be 298 K.	RL	298	~1.0(-1)			2/2
75 SLA/GRA1 Vibrational levels not indicated.	EX	305	(1.24±0.08)(13)			2
76 BID/BRE Vibrational levels not indicated.	EX	300	(1.35±0.22)(13)			2
77 LIL/RIC v≤13. Fast-flow reactor.	EX	150-300	(1.57±0.24)(14)	0	758±144	2
78 KOL Vibrational levels not indicated. Fast-flow reactor.	EX	300	(1.35±0.22)(13)			2
O + CS₂ → SO + CS (a) → S + COS (b) → S₂ + CO (c)						
Oxygen atom + Carbon disulfide						
71 TAK k _a . Step (a) is followed by the very fast reaction: O + CS → CO + S.	EX	298	(1.42±0.20)(12)			2
75 WEI/TIM k _a .	EX	218-293	(1.66±0.23)(13)	0	644±35	2
74 SLA/GIL k _b /(k _a + k _b + k _c).	RL	302	9.3(-2)			2/2
77 GRA/GUT k _b /(k _a + k _b + k _c). Within the given T range, the ratio decreases from 0.098±0.004 to 0.081±0.007.	RL	249-500	(9.8±0.4)(-2)			2/2
77 GRA/GUT k _a + k _b + k _c . Non-linear Arrhenius behaviour. Within the given T range, k increases from 1.75x10 ¹² to 6.75x10 ¹² cm ³ mol ⁻¹ s ⁻¹ .	EX	249-500	(1.75±0.12)(12)			2 1.3
74 SLA/GIL k _a + k _b + k _c .	EX	302	2.41(12)			2
79 HSU/SHA k _c . Flash-photolysis. Laser Resonance- absorption.	EX	298	(3.5±0.5)(10)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + COS → CO + SO (a) → CO ₂ + S (b)						
Oxygen atom + Carbon oxide sulfide						
71 KRE k _a .	RN	300-523	9.82(12)	0	2265	2
71 KRE/SIM k _a .	EX	300-523	9.78(12)	0	2265	2
72 BRE/MIL k _a . Fast-flow technique with EPR detection. P(Total) = 0.45 torr.	EX	297	(7.2±0.4)(9)			2
74 KLE/STI k _a .	EX	263-502	(9.94±0.78)(12)	0	2167±28	2
75 WEI/TIM k _a .	EX	239-404	(1.2±0.2)(13)	0	2149±35	2
78 YOS/SAI k _a . Fast flow-reactor. Microwave Spectroscopy. P = 0.13 torr.	EX	298	(7.1±0.7)(9)			2
80 ROB/SMI k _a . Pulsed laser photolysis of O ₃ in excess N ₂ and in presence of COS. P(Total) = 100 torr.	EX	296	(1.02±0.12)(10)			2
82 TOP k _b . Oxidation of COS behind reflected shock- waves. Time-of-flight Mass-spectrometry. P = (1.3-2.7) atm.	EX	1200-1900	5.01(13)	0	5527±636	2
81 KRU/WAG ¹⁾ k _a + k _b . M = Ar. n = 0 assumed.	EX	298-1900	7.5(13)	0	2755	2
81 KRU/WAG ¹⁾ k _a + k _b . M = Ar. Recommended k. The preexponential factor expressed as: A(T/298) ¹ .	RE	298-1900	7.45(12)	1.0	2057	2
¹⁾ Measurement of O atoms concentration profiles by Resonance-absorption spectroscopy in shock- tube. O atoms generated by decomposition of N ₂ O in Ar.						
O(¹ D) + COS → CO + SO						
Oxygen atom + Carbon oxide sulfide						
75 GAU/SNE k _{ref} : O(¹ D) + O ₂ → O + O ₂ (¹ Σ _g ⁺)	RL	300	(4.1±0.6)			2/2
75 GAU/SNE	RN	300	1.81(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CH ₃ SH → OH + CH ₃ S (a)						
→ H + CH ₃ S(O) (b)						
→ HS(O) + CH ₃ (c)						
→ CH ₃ S(O)H (d)						
Oxygen atom + Methanethiol						
78 KIR/VET	EX	300-661	(8.5±1.0)(12)	0	625±36	2
k _a . Initial step. Fast-flow reactor. Supersonic molecular beam. Mass-spectrometry.						
78 SLA/BAI	EX	254	1.14(12)			2
k _a . Fast flow-reactor. Photoionization Mass-spectrometer. Non-linear Arrhenius behaviour. k increases to 2.59x10 ¹² cm ³ mol ⁻¹ s ⁻¹ at 495 K.						
81 NIP/SIN	EX	298-560	1)	1)	1)	2
k _a . Phase-shift. O generated by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.						
1) The Arrhenius plot for the rate constant of this reaction is sharply curved, but it can be fitted to the empirical expression: $k = (m) + (n),$ where (m) = (9.15±1.02)x10 ¹¹ and (n) = (3.85±2.40)x10 ¹³ exp(-1673±322/T)						
76 SLA/GRA	EX	300	1.14(12)			2
k _b + k _c + k _d .						
O + CN(v=n) → CO + N(⁴ S) (a)						
→ CO† + N(⁴ S) (b)						
→ CO† + N(² D) (c)						
Oxygen atom + Cyanogen						
72 SCH/WOL2	EX	298	8.0(12)			2
k _a . Unreported T assumed to be 298 K. k unchanged from v=0 to v=5, but decreasing to 6.0x10 ¹² cm ³ mol ⁻¹ s ⁻¹ at v=6.						
73 SCH/SCH1	EX	298	1.26(13)			2
k _a . n = 0 to 6.						
73 SCH/SCH1	EX	298	6.31(13)			2
k _a . n = 7.						
75 ALB/HOY	EX	298	(1.2±0.4)(13)			2
k _a . T-independent within the T-range 275-387 K. v = 0.						
77 SCH/WOL	EX	295	(1.1±0.3)(13)			2
k _b + k _c .						
78 SCH/WOL	EX	298	(1.0±0.4)(13)			2
k _b + k _c . Resonance-absorption Spectroscopy.						


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + NCO → NO + CO						
Oxygen atom + Cyanato						
74 SCH/SCH	EX	298	8.91(12)			2
O + HCN → H + OCN (a) → OH + CN (b)						
Oxygen atom + Hydrocyanic acid						
82 ROT/LOE2 ¹⁾	EX	1500-2600	7.23(13)	0	7460	2
k_a .						
82 ROT/LOE2 ¹⁾	RL	1500-2600	1.6			2/2
$(k_a + k_b)/k_a$.						
82 ROT/LOE2 ¹⁾	RN	1500-2600	4.34(13)	0	7460	2
k_b .						
¹⁾ M = Ar. Reaction of O atoms with HCN behind reflected shock-waves. O atoms generated by fast N ₂ O decomposition. Atomic-resonance Absorption-spectrometry. Same data reported in 80 ROT/LOE. [HCN] = (0.62-4.92) × 10 ¹⁵ molec.cm ⁻³ . P = 1275 torr.						
O + CH₃NH₂ → products						
Oxygen atom + Methanamine						
74 KIR/MER	EX	300-450	(2.7±0.3)(12)	0	770±36	2
Flow reactor. Ultrasonic molecular beam. Mass-spectrometer.						
78 ATK/PIT1 ¹⁾	EX	298-440	5.43(12)	0	830±101	2
78 ATK/PIT1 ¹⁾	EX	298	(3.40±0.34)(11)			2
¹⁾ Flash-photolysis. NO ₂ chemilumcence.						
O + CH₃ONO → OH + HCHO + NO						
Oxygen atom + Nitrous acid methyl ester						
75 DAV/THR	EX	300-410	1.4(13)	0	2622±241	2
O + CH₃NO₂ → CH₃O + NO₂ (a) → OH + CH ₂ NO ₂ (b)						
Oxygen atom + Methane, nitro-						
75 CAM/GOO1	EX	295	(1.9±0.3)(9)			2
$k_a + k_b$.						
O + C₂O → CO + CO						
Oxygen atom + Carbon oxide (C ₂ O)						
72 SHA/MAS	EX	300	5.72(13)			2 1.61

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + CH₂C → CO + CH(A²Δ)						
Oxygen atom + Ethynyl						
82 GRE/HOM2 Reaction of the CH ₂ C/O/H system, diluted in N ₂ /He. O atoms generated by reacting N with NO. Discharge-flow. Resonance-fluorescence. P = 2 torr.	EX	298	≈7.0(11)			2
O + CH₂CH → CO + CH₂ (a)						
→ H + CH ₂ C=O → CH ₂ C=O (b)						
→ C=C=O + H ₂ (c)						
Oxygen atom + Ethyne						
73 GAE/GLA k _a . Upper-limit k.	RN	300	≤1.3(11)			2
73 PEE/MAH2 k _a .	EX	1200-1700	5.2(13)	0	1862	2
77 VAN/VAN k _a .	ES	700-1430	6.7(13)	0	2013	2
81 LOE/ROT k _a . Oxydation of CH ₂ CH behind shock-waves. Atomic Resonance-absorption Spectroscopy.	EX	1500-2570	1.20(14)	0	3300	2
81 TSU/HAS k _a . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures, behind reflected shock-waves.	ES	1200-1800	2.00(13)	0	1563	2
82 ROT/LOE2 k _a . M = Ar. Reaction of O atoms with CH ₂ CH behind reflected shock-waves. O atoms generated by fast N ₂ O decomposition. Atomic-Resonance Absorption-spectroscopy. P = 1275 torr. [CH ₂ CH] = (2.46-3.69)×10 ¹⁵ molec.cm ⁻³ . [N ₂ O] = (0.22-2.16)×10 ¹⁵ molec.cm ⁻³ .	EX	1500-2600	1.20(14)	0	3300	2
73 GAE/GLA k _b . M = N ₂ . Limiting high-pressure, upper-limit k.	RN	300	≤1.7(11)			2
81 ALE/ARU k _b . Recording of O and H atoms under jet conditions. Resonance-fluorescence.	EX	298-608	(9.03±0.24)(12)	0	2285±217	2
81 LOE/ROT k _b . M = Ar. Oxidation of Ethyne behind shock-waves. Atomic-Resonance Absorption-Spectroscopy.	EX	1500-2570	4.34(14)	0	6100	2
81 TSU/HAS k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures, behind reflected shock-waves.	ES	1200-1800	2.00(13)	0	1564	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

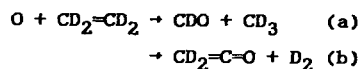
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ROT/LOE2 k _b . M = Ar. Reaction of O atoms with CH=CH behind reflected shock-waves. O atoms generated by fast N ₂ O decomposition. Atomic-resonance Absorption-spectrometry. P = 1275 torr. [CH=CH] = (2.46-3.69)x10 ¹⁵ molec.cm ⁻³ . [N ₂ O] = (0.22-2.16)x10 ¹⁵ molec.cm ⁻³ .	EX	1500-2600	4.34(14)	0	6100	2
71 STU/NIK2 ¹⁾	EX	300	7.89(10)			2 1.1
77 WES/DEH ¹⁾	EX	297	(7.2±0.2)(10)			2
76 HAN/MYE ¹⁾ Discharge-flow . Time-of-flight Mass-spectro-meter.	EX	300-408	1.38(13)	0	1500	2 1.23
81 ALE/ARU ¹⁾ Recording of O and H atoms under jet conditions. Resonance-fluorescence.	EX	298-608	(1.81±0.18)(13)	0	1624±108	2
¹⁾ k _a + k _b .						
73 JON/BAYZ k _a + k _b + k _c .	EX	296	(9.7±1.5)(10)			2
O + CD=CD → CO + CD ₂ (a) → D + CD=C=O → CD ₂ =C=O (b)						
Oxygen atom + Ethyne-d ₂						
71 STU/NIK2 k _a + k _b .	EX	300	7.89(10)			2 1.1
O + CH ₂ =CH ₂ → HCHO + CH ₂ (a) → CHO + CH ₃ (b) → CH ₂ =C=O + H ₂ (c) →  (d)						
Oxygen atom + Ethene						
73 PEE/MAH2 k _a .	ES	1200-1600	2.5(13)	0	2516	2
73 GAE/GLA ¹⁾	ES	300	≈7.0(11)			2
73 HUI ¹⁾	EX	232-500	(3.26±0.18)(12)	0	569±16	2
73 KUR/HUI ¹⁾	EX	298	4.79(11)			2 1.1
73 PEE/MAH2 ¹⁾	EX	1200-1700	2.26(13)	0	1359	2
76 MAN/BRA ¹⁾ Flash-photolysis. Resonance-fluorescence. P(Total) = 5 torr.	EX	298	(4.51±0.24)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 SUG/ISHI ¹⁾ Pulse-radiolysis. Resonance-absorption. Predominant path. P = (50-950) torr.	EX	296	(6.02±1.20)(11)			2
¹⁾ k _b .						
74 PRU/SLA k _b /(k _b + k _c).	RL	300	9.5(-1)			2/2
82 NIC/RAV ²⁾	EX	298	(4.32±0.44)(11)			2
82 NIC/RAV ²⁾ Arrhenius plot is linear below 500 K, but exhibits a curvature above 500 K. Measured k's above 500 K are: 552 K: (1.6±0.2)(12); 695 K: (2.4±0.3)(12); 708 K: (2.3±0.2)(12); 736 K: (2.7±0.3)(12); 811 K: (3.0±0.4)(12); 835 K: (3.5±0.9)(12); 944 K: (4.2±1.2)(12).	EX	298-500	(7.35±3.73)(12)	0	870±190	2
²⁾ k _b + k _c . Flash-photolysis. Resonance- fluorescence. O atoms generated by Flash-photolysis of O ₂ . [CH ₂ =CH ₂] = (0.01-2.0) × 10 ¹⁵ molec.cm ⁻³ . [O] ~ (2-4) × 10 ¹⁰ molec.cm ⁻³ . P(Ar) = 100 torr.						
82 TEM/WAG2 ³⁾ k _b /(k _a + k _b + k _c + k _d). P = 0.75 torr.	RL	298	3.5(-1)			2/2
82 TEM/WAG2 ³⁾ k _b /(k _a + k _b + k _c + k _d). P = 3.0 torr.	RL	298	6.0(-1)			2/2
³⁾ Reaction of O with Ethene in a isothermal dis- charge-flow reactor, in He. LMR-spectrometry.						
74 PRU/SLA k _c .	EX	300	(2.29±0.57)(10)			2
73 GAE/GLA k _d . Limiting high-pressure k. M = N ₂ .	ES	300	≈7.0(11)			2
71 ATK/CVE k _a + k _b + k _c + k _d .	EX	298	(3.0±2.0)(11)			2
71 STU/NIK2 k _a + k _b + k _c + k _d .	EX	300	3.79(1)			2 1.15
72 ATK/CVE k _a + k _b + k _c + k _d .	EX	298-473	8.1(12)	0	976±50	2
72 ATK/CVE k _a + k _b + k _c + k _d .	EX	298	(3.0±0.2)(11)			2
72 DAV/HUI k _a + k _b + k _c + k _d .	EX	232-500	(3.26±0.18)(12)	0	569±16	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 STU/NIK3 $k_a + k_b + k_c + k_d$.	EX	298	(3.76±0.38)(11)			2	
74 ATK/PIT1 $k_a + k_b + k_c + k_d$.	EX	300-392	3.37(12)	0	639±101	2	
74 ATK/PIT2 $k_a + k_b + k_c + k_d$.	EX	301	(4.0±0.4)(11)			2	
74 FUR/ATK $k_a + k_b + k_c + k_d$.	EX	298	(4.3±0.5)(11)			2	
74 MCC $(k_a + k_b + k_c + k_d)/k_{ref}$. k_{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(4.2±1.0)(-2)			2/2	
74 SLA/PRU $k_a + k_b + k_c + k_d$.	EX	300	4.64(12)			2	
76 SIN/CVE $k_a + k_b + k_c + k_d$.	EX	298-480	(6.89±0.89)(12)	0	845±47	2	
77 ATK/PIT1 $k_a + k_b + k_c + k_d$.	EX	298-439	5.56(12)	0	742±101	2	1.1
77 ATK/PIT1 $k_a + k_b + k_c + k_d$.	EX	298	(4.58±0.46)(11)			2	



Oxygen atom + Ethene-d₄

73 KUR/HUI k_a .	EX	298	4.93(11)			2	1.1
72 STU/NIK3 $k_a + k_b$.	EX	298	(3.37±0.34)(11)			2	
82 NIC/RAV ¹⁾ $k_a + k_b$.	EX	298	(4.48±0.38)(11)			2	
82 NIC/RAV ¹⁾ $k_a + k_b$. Arrhenius plot is linear below 500 K, but exhibits a curvature above 500 K. Measured k's above 500 K are: 523 K: (1.5±0.1)(+12); 595 K: (1.8±0.2)(+12); 708 K: (2.3±0.2)(+12); 811 K: (2.6±0.3)(+12).	EX	298-500	(7.35±3.73)(12)	0	870±190	2	

¹⁾ Flash-photolysis. Resonance-fluorescence, O
atoms generated by Flash-photolysis of O₂.

$$[CD_2=CD_2] = (0.01-2.0) \times 10^{15} \text{ molec. cm}^{-3}$$



$$[O] \sim (2-4) \times 10^{10} \text{ molec. cm}^{-3}$$

$$P(\text{Ar}) = 100 \text{ torr.}$$

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O(¹D) + CH₂=CH₂ → products						
Oxygen atom + Ethene						
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. P(Total) = 200 torr. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂	RL	298	(1.8±0.4)			2/2
O + CH₃CH₂ → H + CH₃CHO (a) → CH₃ + HCHO (b)						
Oxygen atom + Ethyl						
79 HOY/SIE3 k _a /k _b . Nozzle reactor. Mass-spectrometry.	RL	298	(5.0±1.0)			2/2
O + CH₃CH₃ → HCHO + H₂ + CH₂ (a) → OH + CH₃CH₂ (b)						
Oxygen atom + Ethane						
71 AVR/KOL1 k _a .	EX	313-523	(1.23±0.60)(12)	0	2164±352	2
71 AVR/KOL1 ¹⁾	EX	313-523	(2.29±1.14)(13)	0	3775±352	2
71 PAP/ASH ¹⁾	EX	300-365	2.75(13)	0	3271±126	2 1.48
80 TAN/KLE ¹⁾	EX	416-1048	(1.12±0.04)(14)	0	3949±36	2
Reaction of O atom with Ethane in a Quartz tube. Flash-photolysis. Discharge-flow. Resonance-fluorescence. [O] = (1.0-3.0) atoms.cm ⁻³ . Pressure-independent k.						
82 CAY/PEE ¹⁾	EX	600-1030	(1.9±0.8)(14)	0	4806±159	2
Discharge flow. Molecular beam sampling. Mass-spectrometry.						
¹⁾ k _b .						
O(¹D) + CH₃CH₃ → OH + CH₃CH₂						
Oxygen atom + Ethane						
74 MIC/PAR k _{ref} : O(¹ D) + (CH ₃) ₄ C → products.	RL	300	(5.12±0.05)(-1)			2/2
76 FLE/HUS	EX	300	(4.39±0.48)(14)			2
81 PRA/PAU Photolysis of O ₂ /CH ₃ CH ₃ mixtures diluted in He. P(O ₂) >15 torr. P(He) = 600 torr. k _{ref} = O(¹ D) + O ₂ → O(³ P) + O ₂	RL	298	(1.24±0.06)(1)			2/2
O + CH=C=O → CO + CO + H						
Oxygen atom + Ethenyl, 2-oxo-						
73 JON/BAY1	EX	298	(1.2±0.3)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + CH₂=C=O → products							
Oxygen atom + Ethenone (Ketene)							
73 JON/BAY2	EX	296	(1.7±0.4)(11)			2	
74 MAC/THR2	EX	293	(3.4±0.3)(11)			2	
The predominant step is: O + CH ₂ =C=O → CHO + CHO							
75 GAF/ATK1 ¹⁾	RL	296	(2.4±0.2)(-2)			2/2	
k _{ref} : O + CH=CHCH ₂ CH ₂ CH ₂ → products.							
75 GAF/ATK1 ¹⁾	RN	296	(2.78±0.35)(11)			2	
Determined relative to the reaction: O + CH=CHCH ₂ CH ₂ CH ₂ → products.							
¹⁾ Competitive technique. Static high-vacuum technique. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography.							
O + CH₃CHO → OH + CH₃CO (a)							
→ OH + CH ₂ CHO (b)							
→ HCHO + H ₂ + CO (c)							
→ CO ₂ + H ₂ + CH ₂ (d)							
Oxygen atom + Acetaldehyde							
71 AVR/KOL2 ¹⁾	EX	373-428	1.60(10)	0	604	2	
74 MAC/THR1 ¹⁾	EX	300	(2.88±0.3)(11)			2	
77 MIC/LEE ¹⁾	EX	298	(2.95±0.30)(11)			2	
Discharge-flow. Resonance-fluorescence.							
77 SIN/IRW ¹⁾	ES	298-472	(7.00±1.40)(12)	0	977±77	2	
Phase-shift.							
81 MOR1 ¹⁾	EX	298	(2.9±0.4)(11)			2	
Discharge-flow. Time-of-flight. Mass-spectrometry. Gas-chromatography.							
¹⁾ k _a .							
77 SIN/IRW	EX	298-472	(7.21±1.49)(12)	0	986±77	2	
k _a + k _b . Phase-shift.							
71 AVR/KOL2	EX	373-428	4.28(12)	0	2919	2	
k _b .							
71 AVR/KOL2	EX	373-428	8.79(10)	0	1158	2	
k _c + k _d .							
O +  → OH + 							
Oxygen atom + Oxirane (Ethylene epoxide)							
78 BOG/HAN ¹⁾	EX	298-691	1.91(12)	0	2642±75	2	1.20
Suggested realistic error limits are: a factor of 3 at 300 K and a factor of 1.5 AT 700 k.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 BOG/HAN ¹⁾	RL	482-691	(9.0±2.0)(1)	0	-735±116	2/2	
$k_{\text{ref}}: \text{O} + \begin{array}{c} \text{O} \\ \diagup \quad \diagdown \\ \text{D} \quad \text{D} \end{array} \rightarrow \text{OD} + \begin{array}{c} \text{O} \\ \diagdown \quad \diagup \\ \text{D} \quad \text{D} \end{array}$							
¹⁾ Discharge-flow. Mass-spectrometry. Photometry.							
$\text{O} + \text{HC(O)OCH}_3 \rightarrow \text{OH} + \text{C(O)OCH}_3$							
Oxygen atom + Formic acid methyl ester (Methyl formate)							
81 MOR1	EX	298	(5.6±1.1)(9)				2
Discharge-flow. Mass-spectrometry.							
82 FAU/HOY	EX	298	(6.4±2.5)(8)				2
Reaction of O with HCOOCH ₃ in a flow-system.							
P = (4-8) torr. [O] = (2.2-6.6) × 10 ¹⁴ molec.cm ⁻³ .							
$\text{O} + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{OH} + \text{CH}_3\text{CHOH} \quad (\text{a})$							
$\quad \quad \quad \rightarrow \text{OH} + \text{CH}_2\text{CH}_2\text{OH} \quad (\text{b})$							
$\quad \quad \quad \rightarrow \text{OH} + \text{CH}_3\text{CH}_2\text{O} \quad (\text{c})$							
$\quad \quad \quad \rightarrow \text{HCHO} + \text{CH}_2 + \text{H}_2\text{O} \quad (\text{d})$							
$\quad \quad \quad \rightarrow \text{H}_2\text{O} + \text{CH}_3\text{CHO} \quad (\text{e})$							
Oxygen atom + Ethanol							
76 OWE/ROS	EX	301-439	4.17(8)	0	758±204	2	1.12
k _a . Flow reactor.							
71 AVR/KOL2 ¹⁾	EX	343-413	1.87(13)	0	2944		2
81 WAS ¹⁾	EX	298	(1.02±0.18)(11)				2
Fast-flow reactor. Mass-spectrometry. O atoms generated by a He/O ₂ mixture, by a microwave-discharge.							
P(Total) = (3.73-3.88) torr.							
¹⁾ k _a + k _b + k _c .							
71 AVR/KOL2	EX	343-523	3.43(11)	0	1334		2
k _d .							
71 AVR/KOL2	EX	343-413	7.47(11)	0	1485		2
k _e .							
$\text{O} + \text{CD}_3\text{CD}_2\text{OH} \rightarrow \text{OD} + \text{CD}_3\text{CDOH} \quad (\text{a})$							
$\quad \quad \quad \rightarrow \text{OD} + \text{CD}_2\text{CD}_2\text{OH} \quad (\text{b})$							
$\quad \quad \quad \rightarrow \text{OH} + \text{CD}_3\text{CD}_2\text{O} \quad (\text{c})$							
Oxygen atom + Ethan-d ₅ -ol							
81 WAS	EX	298	(6.62±2.41)(10)				2
k _a + k _b + k _c . Fast-flow reactor. Photoionization Mass-spectrometry. O atoms generated in a He/O ₂ mixture, in a microwave-discharge.							
P(Total) = 3.73 mtorr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + (CH₃)₂O → OH + CH₂OCH₃							
Oxygen atom + Methane, oxybis- (Dimethyl ether)							
72 LEF/MEA	EX	217-366	(5.0±1.0)(12)	0	1434±101	2	
82 FAU/HOY	EX	298	(2.3±0.7)(10)			2	
Reaction of O with HCOOCH ₃ in a flow-system. [O] = (2.2-6.0) × 10 ¹⁴ molec.cm ⁻³ . P = (41-101) torr.							
O + \triangle → SO + CH₂=CH₂							
Oxygen atom + Thiirane (Ethylene episulfide)							
76 LEE/TIM	EX	298-478	(8.07±0.54)(12)	0	18±20	2	
O + CH₃CH₂SH → OH + CH₃CH₂S (a)							
→ HS(O) + CH ₃ CH ₂ (b)							
→ H + CH ₃ CH ₂ S(O) (c)							
→ CH ₃ CH ₂ S(O)H (d)							
Oxygen atom + Ethanethiol (Ethyl mercaptan)							
78 KIR/VET	EX	304-421	(5.75±0.3)(12)	0	391±18	2	
k _a . Initial step in a suggested mechanism. Supersonic molecular beam. Fast flow-reactor. Mass-spectrometry.							
78 SLA/BAI	EX	257	1.93(12)			2	
k _a . Fast flow. Photoionization Mass-spectrometry. Non-linear Arrhenius behaviour. k increasing to 3.19 × 10 ¹² cm ³ mol ⁻¹ s ⁻¹ at 495 K.							
81 NIP/SIN	EX	298-560	1)	1)	1)	2	
k _a . Phase-shift technique. O atoms generated by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.							
1) The Arrhenius plot for k of this reaction is sharply curved, but it can be fitted to the empirical expression: k = (m) + (n), where: (m) = (1.37±0.07) × 10 ¹² and (n) = (8.73±4.46) × 10 ¹³ exp(-2075±268/T)							
76 SLA/GRA	EX	300	1.69(12)			2	
k _b + k _c + k _d .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + (CH₃)₂S → CH₃S(O) + CH₃ (a)						
→ CH₃O + CH₃S (b)						
Oxygen atom + Methane, thiobis- (Dimethyl sulfide)						
78 SLA/BAI	EX	252	3.79(13)			2
k _a . Fast flow. Photoionization Mass-spectrometry. Possible non-linear Arrhenius behaviour. k decreasing to: 2.17x10 ¹³ cm ³ mol ⁻¹ s ⁻¹ at 493 K.						
80 LEE/TAN1	EX	272-472	(7.71±0.72)(12)	0	-404±30	2
k _a . Fast-flow. Resonance-fluorescence.						
81 NIP/SIN	EX	298-560	(6.69±0.72)(12)	0	-460±41	2
k _a . Phase-shift. O atoms formed by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.						
74 CAD/WIC ¹⁾	EX	300	3.3(11)			2
76 LEE/TIM ¹⁾	EX	268-424	(8.55±0.42)(12)	0	-366±16	2
76 SLA/GRA ¹⁾	EX	300	3.79(13)			2
¹⁾ k _a + k _b .						
O + CH₃SSCH₃ → products						
Oxygen atom + Disulfide, dimethyl-						
80 LEE/TAN2	EX	270-329	(1.28±0.13)(14)	0	0	2
Discharge fast-flow. Resonance-fluorescence. P = (0.52-2.60) torr.						
81 NIP/SIN	EX	298-560	(2.62±0.42)(13)	0	-251±61	2
Phase-shift. O atoms formed by Hg-photosensitized decomposition of N ₂ O. Gas-chromatography.						
O + CH₃CN → OCN + CH₃						
Oxygen atom + Acetonitrile						
77 BON/TIM	EX	383-500	(4.38±1.05)(11)	0	2401±101	2
77 BON/TIM ¹⁾	RL	383	(1.2±0.3)			2/2
77 BON/TIM ¹⁾	RL	423	(1.5±0.6)			2/2
¹⁾ k _{ref} : O + CD ₃ CN → OCN + CD ₃						
O + CH₃CH₂NH₂ → products						
Oxygen atom + Ethanamine						
74 KIR/MER	EX	300-450	(3.9±0.3)(12)	0	529±24	2
Flow reactor. Ultrasonic molecular beam. Mass-spectrometer.						
78 ATK/PIT1 ¹⁾	EX	298-440	6.81(12)	0	642±101	2
78 ATK/PIT1 ¹⁾	EX	299	(8.01±0.84)(11)			2
¹⁾ Flash-photolysis. NO ₂ chemiluminescence.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
O + (CH₃)₂NH → products							
Oxygen atom + Methanamine, N-methyl-							
74 KIR/MER Ultrasonic molecular beam. Mass-spectrometer. Flow reactor.	EX	300	3.2(12)			2	
78 ATK/PIT1 ¹⁾	EX	298-440	9.15(12)	0	277±101	2	
78 ATK/PIT1 ¹⁾	EX	298	(3.69±0.37)(12)			2	
¹⁾ NO ₂ chemiluminescence. Flash-photolysis.							
O + CH₃CH₂ONO → OH + CH₃CHO + NO							
Oxygen atom + Nitrous acid ethyl ester							
75 DAV/THR	EX	300-410	2.6(13)	0	2442±241	2	
O + O=C=C=C=O → CO + CO + CO							
Oxygen atom + 1,2-Propadiene-1,3-dione							
74 PIL/WAG	EX	250-450	(1.0±0.2)(13)	0	1100±170	2	
O(¹D) + O=C=C=C=O → CO + CO + CO							
Oxygen atom + 1,2-Propadiene-1,3-dione							
73 HEI/HUS2	EX	300	(2.41±0.24)(14)			2	
O + CH₃C≡CH → CO + CH₃CH (a) → H + [C₃H₃O] (b)							
Oxygen atom + 1-Propyne							
73 HER <i>k</i> _a . Assumed to pass through a vibrationally excited intermediate: 2-Methyloxirene.	EX	275-360	1.6(13)	0	1010	2	
74 HER/WAG <i>k</i> _a . Isothermal flow-system. P = (5-40) torr.	EX	290-360	1.3(13)	0	1007±201	2	
81 ALE/DUB ¹⁾ <i>k</i> _b .	EX	295-545	(3.61±1.20)(12)	0	1323±217	2	
81 ALE/DUB ¹⁾ <i>k</i> _{overall} .	EX	295-545	(8.43±2.42)(12)	0	866±108	2	
¹⁾ Recording of O and H atoms under jet conditions. Resonance-fluorescence.							
75 ARR/COX <i>k</i> _{overall} .	EX	298-600	(1.39±0.36)(13)	0	981±352	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O + CH_2=C=CH_2 \rightarrow CO + CH_2=CH_2$ (a) $\rightarrow H + [C_3H_3O]$ (b)							
Oxygen atom + 1,2-Propadiene (Allene)							
72 HER/WAG k_a .	EX	275-375	7.8(12)	0	805	2	1.3
73 HER k_a . Assumed to pass through a vibrationally excited intermediate:	EX	275-360	7.8(12)	0	806	2	
Methyleneoxirane.							
74 HAV 1) k_{ref} : $O + CH_3CH_2CH=CH_2 \rightarrow$ products.	RL	298	6.5(-1)				2/2
74 HAV 1) k_{ref} : $O + (CH_3)_2C=CH_2 \rightarrow$ products.	RL	298	1.97(-1)				2/2
1) k_a/k_{ref} . Two vibrationally excited precursors are suggested:							
Methyleneoxirane, or Cyclopropanone.							
80 ALE/ARU2 k_b . Resonance-fluorescence.	EX	295-860	6.63(12)	0	1535±151	2	
77 ATK/PIT2 2)	EX	297-439	1.23(13)	0	883±101	2	1.1
77 ATK/PIT2 2)	EX	298	(6.44±0.66)(11)			2	
79 NIP/SIN 2) Modulated, Hg-sensitized N_2O decomposition. Phase-shift.	EX	297-574	(1.80±0.25)(13)	0	941±54	2	
80 ALE/ARU2 2) Resonance-fluorescence.	EX	295-860	1.02(13)	0	956±101	2	
2) $k_{overall}$.							
$O + CH_3CH=CH_2 \rightarrow$ <div style="display: inline-block; vertical-align: middle;"> $\begin{array}{c} O^\dagger \\ \triangle \\ CH_2 \end{array}$ </div> (a)							
$\rightarrow OH + CH_2CH=CH_2$ (b)							
$\rightarrow CH_3CHO + CH_2:$ (c)							
$\rightarrow HCHO + H_2 + CH_2=C:$ (d)							
Oxygen atom + 1-Propene							
72 KUR1 k_a , or possibly k_b .	EX	201-424	(2.51±0.20)(12)	0	38±22	2	
73 GAE/GLA k_a . $M = N_2$. Estimated k.	RN	300	≈2.9(12)			2	
73 HER k_a .	EX	275-360	4.2(12)	0	253	2	
71 AVR/KOL1 k_b .	EX	373-583	7.23(12)	0	2718	2	
71 AVR/KOL1 k_c .	EX	361-483	5.06(10)	0	755	2	



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 AVR/KOL1 k _d .	EX	361-483	5.42(11)	0	1258	2	
71 ATK/CVE ¹)	EX	298	(1.18±0.06)(12)			2	
71 STU/NIK2 ¹)	EX	300	2.17(12)			2	1.1
72 ATK/CVE ¹)	EX	298-473	6.7(12)	0	518±50	2	
72 ATK/CVE ¹)	EX	298	(1.18±0.06)(12)			2	
73 GAE/GLA ¹)	RN	300	≈2.7(12)			2	
74 ATK/PIT1 ¹)	EX	300-392	2.08(12)	0	0±151	2	
74 ATK/PIT2 ¹)	EX	300	(2.01±0.22)(12)			2	
74 FUR/ATK ¹)	EX	298	(2.02±0.17)(12)			2	
75 GAF/ATK1 ¹)	RN	296	2.10(12)			2	
76 SIN/CVE ¹)	EX	298-480	(7.58±0.42)(12)	0	363±20	2	
77 ATK/PIT1 ¹)	EX	298-439	6.32(12)	0	259±101	2	1.1
77 ATK/PIT1 ¹)	EX	299	(2.69±0.27)(12)			2	
77 MIC/LEE ¹) Resonance-fluorescence. Discharge-flow.	EX	298	(2.38±0.25)(12)			2	
80 SUG/ISH1 ¹) Resonance-absorption. Pulse-radiolysis. P = (50-950) torr.	EX	296	(2.83±0.18)(12)			2	
82 BIE/HAR ¹) Photoionization Mass-spectrometry. Discharge-flow system. P(Total) ~ 2 torr.	EX	298	(2.65±0.36)(12)			2	
¹) k _{overall} .							
74 MCC k _{overall} /k _{ref} . k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(2.0±0.5)(-1)			2/2	
75 GAF/ATK1 k _{overall} /k _{ref} . Competitive technique. Static system. O-atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k _{ref} : O + CH=CHCH ₂ CH ₂ CH ₂ → products.	RL	296	(1.81±0.10)(-1)			2/2	
O(¹ D) + CH ₃ CH=CH ₂ → products Oxygen atom + 1-Propene							
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ P(Total) = 200 torr.	RL	298	(5.0±1.0)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O + \triangle \rightarrow OH + \triangle$						
Oxygen atom + Cyclopropane						
76 LEE	EX	298-478	(3.31±0.42)(12)	0	3120±60	2
$O + CH_3CH_2CH_2 \rightarrow H + CH_3CH_2CHO$ (a) $\rightarrow HCHO + CH_3CH_2$ (b)						
Oxygen atom + Propyl						
79 HOY/SIE3 k_a/k_b . Low pressure nozzle reactor. Mass-spectrometry.	RL	298	(6.0±1.5)			2/2
$O + (CH_3)_2CH \rightarrow H + (CH_3)_2CO$ (a) $\rightarrow CH_3 + CH_3CHO$ (b)						
Oxygen atom + Ethyl, 1-methyl- (Isopropyl)						
79 HOY/SIE3 k_a/k_b . Low pressure nozzle reactor. Mass-spectrometry.	RL	298	(1.0±0.2)			2/2
$O + CH_3CH_2CH_3 \rightarrow OH + (CH_3)_2CH$ (a) $\rightarrow OH + CH_3CH_2CH_2$ (b)						
Oxygen atom + Propane						
75 HAR/BUR $k_a + k_b$.	EX	329	(3.9±0.7)(10)			2
81 JEW/HOL $k_a + k_b$. Discharge-flow reactor. O atoms produced by reacting N with NO. Gas-chromatography.	EX	306	(4.7±0.8)(9)			2
$O(^1D) + CH_3CH_2CH_3 \rightarrow OH + (CH_3)_2CH$ (a) $\rightarrow OH + CH_3CH_2CH_2$ (b)						
Oxygen atom + Propane						
75 GAU/SNE ¹⁾	RN	300	4.82(14)			2
76 FLE/HUS ¹⁾ ¹⁾ $k_a + k_b$.	EX	300	(5.72±0.60)(14)			2
74 MIC/PAR $(k_a + k_b)/k_{ref}$. k_{ref} : $O(^1D) + (CH_3)_4C \rightarrow$ products.	RL	300	(6.52±0.27)(-1)			2/2
75 GAU/SNE $(k_a + k_b)/k_{ref}$. k_{ref} : $O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$	RL	300	(1.08±0.20)(1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 PRA/PAU ($k_a + k_b$)/ k_{ref} . Photolysis of O ₂ /Propane mixtures in He. P(O ₂) >15 torr. P(He) = 600 torr. $k_{ref} = O(^1D) + O_2 \rightarrow O(^3P) + O_2$	RL	298	(1.34±0.04)(1)				2/2
O + CH₂=CHCHO → products							
Oxygen atom + 2-Propenal (Acrolein)							
72 CAD/LIN	EX	300-480	(4.7±1.6)(12)	0	1007±151	2	
75 GAF/ATK1	RL	296	(2.0±0.2)(-2)				2/2
k_{ref} : O +  → products.							
75 GAF/ATK1	RN	296	(2.3±0.23)(11)			2	
75 GAF/ATK2	RL	296	(2.0±0.2)(-2)				2/2
75 GAF/ATK2 ¹⁾	RN	296-423	1.4(13)	0	1208±136	2	
75 GAF/ATK2 ¹⁾	RN	296	(2.32±0.23)(11)			2	
¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k determined relative to the reaction:							
O +  → products,							
and placed on an absolute basis by using the k expression from the literature, for the reaction:							
O + CH ₃ CH=CH ₂ → products. Supersedes 75 GAF/ATK1.							
O + CH₂=CHOCH₃ → products							
Oxygen atom + Ethene, methoxy-							
77 ATK/PIT2	EX	297-439	3.81(12)	0	-38±101	2	1.1
77 ATK/PIT2	EX	297	(4.30±0.43)(12)			2	
O + CH₃CH₂CHO → OH + CH₃CH₂C (a)							
→ OH + CH ₃ CHCHO (b)							
→ OH + CH ₂ CH ₂ CHO (c)							
Oxygen atom + Propanal							
72 CAD/LIN	EX	300-480	(8.5±2.8)(13)	0	1912±252	2	
$k_a + k_b + k_c$.							
77 SIN/IRW ¹⁾	ES	298-472	(5.67±0.51)(12)	0	777±31	2	
k_a .							
77 SIN/IRW ¹⁾	EX	298-472	(7.78±0.75)(12)	0	869±33	2	
$k_a + k_b + k_c$.							
¹⁾ Phase-shift technique.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + (CH₃)₂CO → OH + CH₃COCH₂							
Oxygen atom + 2-Propanone							
72 AZA/GYU	EX	873	8.43(10)			2	
76 AMB/BRA	EX	298-621	4.27(12)	0	2863±84	2	1.26
Discharge-flow. ESR detection.							
76 LEE	EX	298-478	(1.86±0.37)(12)	0	2536±101	2	
77 LEE/TIM	EX	298-478	(1.9±0.4)(12)	0	2536±91	2	
82 FAU/HOY	EX	298	(6.8±2.9)(8)			2	
Reaction of O with HCOOCH ₃ in a flow-system.							
[O] = (3.3-4.0)×10 ¹⁴ molec.cm ⁻³ .							
P = (5-10) torr.							
O + HC(O)OCH₂CH₃ → OH + C(O)OCH₂CH₃							
Oxygen atom + Formic acid ethyl ester (Ethyl formate)							
82 FAU/HOY	EX	298	(1.0±0.4)(9)			2	
Reaction of O with HCOOCH ₃ in a flow-system.							
[O] = (2.2-7.2)×10 ¹⁴ molec.cm ⁻³ .							
P = (5-17) torr.							
O + CH₃C(O)OCH₃ → OH + CH₃C(O)OCH₂ (a)							
→ OH + CH₂C(O)OCH₃ (b)							
Oxygen atom + Acetic acid methyl ester (Methyl acetate)							
82 FAU/HOY	EX	298	(4.9±2.0)(8)			2	
k _a + k _b . Reaction of O with HCOOCH ₃							
in a flow-system. P = (4-8) torr.							
[O] = (3.3-7.8)×10 ¹⁴ molec.cm ⁻³ .							
O + CH₃CH₂CH₂OH → OH + CH₃CH₂CHOH (a)							
→ OH + CH₃CH₂CH₂O (b)							
Oxygen atom + 1-Propanol							
79 AYU/ROS	EX	463-308	7.92(11)	0	1500±165	2	1.10
k _a + k _b . Initial steps in a suggested mechanism.							
Fast-flow system. Microwave-discharge.							
Gas-chromatography. Mass-spectrometry.							
O + (CH₃)₂CHOH → OH + (CH₃)₂COH (a)							
→ OH + (CH₃)₂CHO (b)							
Oxygen atom + 2-Propanol							
79 AYU/ROS	EX	306-428	3.19(11)	0	1100±143	2	1.07
k _a + k _b . Initial steps in a suggested mechanism.							
Gast-flow system. Microwave-discharge.							
Gas-chromatography. Mass-spectrometry.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err. factor
O + CH₃CH₂CH₂SH → OH + CH₃CH₂CH₂S							
Oxygen atom + 1-Propanethiol (Propyl mercaptan)							
78 KIR/VET Initial step in a suggested mechanism. Supersonic molecular beam. Fast-flow reactor. Mass-spectrometry.	EX	303-421	(8.33±0.54)(12)	0	494±22	2	
O + (CH₃)₃N → products							
Oxygen atom + Methanamine, N,N-dimethyl-							
74 KIR/MER Ultrasonic molecular beam. Mass-spectrometer. Flow reactor.	EX	300	9.4(12)			2	
78 ATK/PIT1 ¹⁾	EX	298-440	6.50(12)	0	209±101	2	
78 ATK/PIT1 ¹⁾	EX	298	(1.33±0.13)(13)			2	
¹⁾ NO ₂ chemiluminescence. Flash-photolysis.							
O + CH=CC=CH → products							
Oxygen atom + 1,3-Butadiyne							
73 JON/BAY2	EX	296	(1.6±0.5)(12)			2	
75 HOM/SCH	EX	297-343	8.0(13)	0	1230	2	
O + CH₂=CHC=CH → products							
Oxygen atom + 1-Buten-3-yne							
75 HOM/SCH	EX	295	(2.95±0.10)(12)			2	
O + CH₃CH₂C≡CH → CO + CH₃CH=CH₂							
Oxygen atom + 1-Butyne							
75 HER/WAG1	EX	290-357	1.7(13)	0	800	2	
77 UMS/LIN CO laser resonant absorption. NO ₂ Flash-photolysis.	EX	298	5.0(11)			2	
O + CH₃C≡CCH₃ → CO + CH₃CH=CH₂							
Oxygen atom + 2-Butyne							
75 HER/WAG2	ES	290-360	6.0(13)	0	900	2	
77 UMS/LIN CO laser resonant absorption. NO ₂ Flash-photolysis.	EX	298	1.6(12)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + CH₃CH=C=CH₂ → products							
Oxygen atom + 1,2-Butadiene							
74 HAV	RL	298	1.39				2/2
k _{ref} : O + CH ₃ CH ₂ CH=CH ₂ → products.							
74 HAV	RL	298	4.3(-1)				2/2
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.							
O + CH₂=CHCH=CH₂ → products							
Oxygen atom + 1,3-Butadiene							
74 MCC	RL	298	(9.6±3.5)(-1)				2/2
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.							
77 ATK/PIT2	EX	297-439	1.36(13)	0	53±101	2	1.1
77 ATK/PIT2	EX	297	(1.17±0.11)(13)			2	
79 NIP/SIN	EX	299-488	(1.25±0.13)(13)	0	0	2	
Hg-sensitized N ₂ O decomposition. Phase-shift.							
80 SUG/ISH1	EX	296	(1.20±0.12)(13)			2	
Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.							
O + CH₃CH₂CH=CH₂ → products							
Oxygen atom + 1-Butene							
71 ATK/CVE	EX	298	(1.55±0.12)(12)			2	
71 HUI/HER	EX	259-493	(8.79±0.90)(12)	0	382±30	2	
72 ATK/CVE	EX	298-473	6.1(12)	0	408±50	2	
72 ATK/CVE	EX	298	(1.55±0.12)(12)			2	
72 HUI/HER2	EX	190-491	¹⁾ ¹⁾		¹⁾	2	1.6
Flash-photolysis. Resonance-fluorescence.							
1) Curved Arrhenius plot. Authors give two additive empirical exponential terms: k _a = (2.23±1.08) × 10 ¹² exp(-25±105/T) and k _b = (9.64±5.42) × 10 ¹² exp(-991±216/T) in units of cm ³ mol ⁻¹ s ⁻¹ . They ascribe k _a O-atom addition and k _b to H-abstraction.							
74 FUR/ATK	EX	298	(2.40±0.32)(12)			2	
74 HAV	RL	298	2.3(-1)				2/2
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.							
74 MCC	RL	298	(1.8±0.7)(-1)				2/2
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.							
76 SIN/CVE	EX	298-480	(7.21±0.44)(12)	0	333±23	2	
77 ATK/PIT1	EX	298-439	8.37(12)	0	335±101	2	1.1
77 ATK/PIT1	EX	299	(2.73±0.28)(12)			2	



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 SUG/ISH1 Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(2.83±0.30)(12)			2	
O + cis-CH₃CH=CHCH₃ → products							
Oxygen atom + 2-Butene, (Z)-							
73 DAV/HUI	EX	268-443	(5.84±0.58)(12)	0	-161±32	2	
74 FUR/ATK	EX	298	(9.00±1.76)(12)			2	
74 HAV	RL	298	9.5(-1)			2/2	
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.							
74 MCC	RL	298	(7.9±2.5)(-1)			2/2	
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.							
76 SIN/CVE	EX	298-480	(6.68±0.23)(12)	0	-135±13	2	
77 ATK/PIT1	EX	298-439	7.29(12)	0	-118±101	2	1.1
77 ATK/PIT1	EX	299	(1.09±0.11)(13)			2	
80 SUG/ISH1 Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(1.20±0.18)(13)			2	
O(¹D) + cis-CH₃CH=CHCH₃ → products							
Oxygen atom + 2-Butene, (Z)-							
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ P(Total) = 200 torr.	RL	298	(7.2±1.5)			2/2	
O + trans-CH₃CH=CHCH₃ → products							
Oxygen atom + 2-Butene, (E)-							
74 MCC k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(1.25±0.35)			2/2	
77 ATK/PIT1	EX	298-439	1.36(13)	0	-10±101	2	1.1
77 ATK/PIT1	EX	299	(1.42±0.14)(13)			2	
80 SUG/ISH1 Pulse-radiolysis. Resonance-absorption. P = (50-950) torr.	EX	296	(1.39±0.18)(13)			2	
O(¹D) + trans-CH₃CH=CHCH₃ → products							
Oxygen atom + 2-Butene, (E)-							
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂ P(Total) = 200 torr.	RL	298	(4.9±1.0)			2/2	


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + (CH₃)₂C=CH₂ → products							
Oxygen atom + 1-Propene, 2-methyl-							
71 ATK/CVE	EX	298	(6.2±1.5)(12)			2	
72 ATK/CVE	EX	298-473	6.3(12)	0	0±201	2	
72 ATK/CVE	EX	298	(6.2±1.5)(12)			2	
74 FUR/ATK	EX	298	(9.85±1.34)(12)			2	
76 SIN/CVE	EX	298-480	(8.74±0.53)(12)	0	-51±22	2	
77 ATK/PIT1	EX	298-439	1.06(13)	0	43±101	2	1.1
77 ATK/PIT1	EX	299	(9.22±0.11)(12)			2	
80 SUG/ISH1	EX	296	(1.02±0.12)(13)			2	
Pulse-radiolysis. Resonance-absorption.							
P = (50-950) torr.							
O(¹D) + (CH₃)C=CH₂ → products							
Oxygen atom + 1-Propene, 2-methyl-							
79 KAJ/FUE	RL	298	(3.7±1.0)			2/2	
N ₂ O photolysis. Gas-chromatography.							
P(Total) = 200 torr.							
k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂							
O + (CH₃)₂C=CHD → products							
Oxygen atom + 1-Propene-1-d ₁ , 2-methyl-							
76 HAV/HUN	RL	298-302	(1.03±0.01)	0	0	2/2	
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.							
O + (CH₃)₂C=CD₂ → products							
Oxygen atom + 1-Propene, 1,1-d ₂ , 2-methyl-							
76 HAV/HUN	RL	298-302	(1.05±0.01)	0	0	2/2	
k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.							
O + (CH₃)₂CBCH₂ → H + (CH₃)₂CBCHO (a) → HCHO + (CH₃)₂CB (b)							
Oxygen atom + Propyl, 2-methyl-							
79 HOY/SIE3	RL	298	(7.0±2.0)			2/2	
k _a /k _b . Low pressure nozzle reactor.							
O + (CH₃)₃C → OH + (CH₃)₂C=CH₂ (a) → CH₃ + (CH₃)₂CO (b)							
Oxygen atom + Ethyl, 1,1-dimethyl-							
80 WAS/BAY	RN	297	(5.24±1.14)(14)			2	
k _a + k _b . Fast-flow reactor system. Photoionization Mass-spectrometer. k measurements by Stern-Volmer plots. P(Total) = (1.8-5.7) torr.							


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O + CH_3CH_2CH_2CH_3 \rightarrow OH + CH_3CH_2CH_2CH_2$ (a) $\rightarrow OH + CH_3CH_2CHCH_3$ (b)							
Oxygen atom + Butane							
71 PAF/ASH ¹⁾	EX	300-365	1.66(13)	0	2280±121	2	1.45
74 ATK/PIT2 ¹⁾	EX	301	(1.88±0.20)(10)			2	
77 ATK/PER1 ¹⁾	EX	298-439	1.51(13)	0	2099±151	2	
77 ATK/PER1 ¹⁾	EX	298	(1.32±0.24)(10)			2	
¹⁾ k _a + k _b .							
O(¹ D) + CH ₃ CH ₂ CH ₂ CH ₃ → products							
Oxygen atom + Butane							
74 MIC/PAR	RL	300	(8.63±0.33)(-1)				2/2
k _{ref} : O(¹ D) + (CH ₃) ₄ C → products.							
O + (CH ₃) ₃ CH → OH + (CH ₃) ₃ C (a) → OH + (CH ₃) ₂ CHCH ₂ (b)							
Oxygen atom + Propane, 2-methyl-							
80 WAS/BAY	EX	297	(6.02±1.20)(10)			2	
k _a + k _b . Fast-flow. Photoionization Mass-spectrometer. P(Total) = (1.8-5.7) torr.							
82 JEW/HOL	EX	307	(7.9±1.4)(10)			2	
k _a + k _b . Reaction of O with Isobutane. Discharge-flow. Gas-chromatography. P = (2-4) torr.							
O + CH ₃ CH=CHCHO → products							
Oxygen atom + 2-Butenal (Crotonaldehyde)							
74 CAD/WIC	EX	~300	2.0(13)	0	1158	2	
74 CAD/WIC	EX	300	5.0(11)			2	
75 GAF/ATK1	RL	296	(4.4±0.5)(-2)				2/2
k _{ref} : O +  → products.							
75 GAF/ATK1	RN	296	(5.10±0.58)(11)			2	
75 GAF/ATK2	RL	296	(4.4±0.5)(-2)				2/2
75 GAF/ATK2 ¹⁾	RN	296-423	1.5(13)	0	996±65	2	
75 GAF/ATK2 ¹⁾	RN	296	(5.10±0.58)(11)			2	
¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k determined relative to the reaction:							
O +  → products,							



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
and placed on an absolute basis by using the k expression from the literature, for the reaction: O + CH ₃ CH=CH ₂ → products. Supersedes 75 GAF/ATK1.						
O + CH ₃ CH ₂ CH ₂ CHO → OH + CH ₃ CH ₂ CH ₂ CO (a)						
→ OH + CH ₃ CH ₂ CHCHO (b)						
→ OH + CH ₃ CHCH ₂ CHO (c)						
→ OH + CH ₂ CH ₂ CH ₂ CHO (d)						
Oxygen atom + Butanal						
74 JAF/WAN ¹⁾	ES	298	1.5(11)			2
77 SIN/IRW ¹⁾	ES	298-472	(6.23±0.13)(12)	0	719±8	2
Phase-shift.						
¹⁾ k _a .						
77 SIN/IRW	EX	298-472	(9.99±0.56)(12)	0	857±20	2
k _a + k _b + k _c + k _d .						
Phase-shift.						
O + (CH ₃) ₂ CHCHO → OH + (CH ₃) ₂ CHCO (a)						
→ OH + (CH ₃) ₂ CCHO (b)						
→ OH + CH ₂ CH(CH ₃)CHO (c)						
Oxygen atom + Propanal, 2-methyl-						
77 SIN/IRW	ES	298-472	(7.18±0.87)(12)	0	700±43	2
k _a .						
Phase-shift.						
77 SIN/IRW	EX	298-472	(7.92±1.02)(12)	0	727±46	2
k _a + k _b + k _c .						
Phase-shift.						
O + (CH ₃ CH ₂) ₂ O → OH + CH ₃ CHOCH ₂ CH ₃ (a)						
→ OH + CH ₂ CH ₂ OCH ₂ CH ₃ (b)						
Oxygen atom + Ethane, 1,1'-oxybis-						
82 FAU/HOY	EX	298	(6.7±3.5)(10)			2
k _a + k _b . Reaction of O with HCOOCH ₃ in a flow-system. P = (12-50) torr.						
[O] = (3.3-4.0) × 10 ¹⁴ molec. cm ⁻³ .						
O +  → products						
Oxygen atom + Thiophene						
81 LEE/TAN	EX	262-448	(2.01±0.20)(13)	0	569±30	2
Discharge-flow system. Resonance-fluorescence.						
[O] ₀ = (0.5-1.0) × 10 ¹¹ atoms. cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O + CH₃CH₂CH₂CH₂SH → OH + CH₃CH₂CH₂CH₂S							
Oxygen atom + 1-Butanethiol (Butyl mercaptan)							
78 KIR/VET Initial step in a suggested mechanism. Supersonic molecular beam. Fast flow-reactor. Mass-spectrometry.	EX	306-419	(5.78±0.33)(12)	0	321±19	2	
O + NCC≡CCN → NCCO + CCN							
Oxygen atom + 2-Butynedinitrile							
72 HAN/OBE1 Predominant first step. Discharge-flow reactor. Time-of-flight Mass-spectrometry. P(Total) = 137 torr.	EX	298	(6.63±1.81)(8)			2	
76 HAN/MYE Predominant first step. Discharge-flow reactor. Time-of-flight Mass-spectrometry. P = (0.73-1.10) torr.	EX	300-408	7.94(12)	0	2768±554	2	5.01
O + CH₃CH₂CH₂C≡CH → CO† + CH₃CH₂CH₂CH:							
Oxygen atom + 1-Pentyne							
80 SHA/BUR Flash-photolysis. CO laser Resonance-absorption.	EX	293	(4.9±0.6)(11)			2	
O + (CH₃)₂C=C=CH₂ → products							
Oxygen atom + 1,2-Butadiene, 3-methyl-							
74 HAV k _{ref} : O + (CH ₃) ₂ C=CHCH ₃ → products.	RL	298	7.6(-1)			2/2	
O +  → products							
Oxygen atom + Cyclopentene							
75 GAF/ATK2 Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k placed on an absolute basis by using the k expression from the literature, for the reaction: O + CH ₃ CH=CH ₂ → products. Supersedes 75 GAF/ATK1.	RN	296-423	5.6(12)	0	-216±40	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

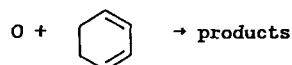
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k units factor	err. factor
O +  → products							
Oxygen atom + Spiropentane							
72 HUI/HER3 Discharge-flow. Mass-spectrometry.	EX	337-652	3.98(13)	0	2890±100	2	1.26
O + CH ₃ CH ₂ CH ₂ CH=CH ₂ → products							
Oxygen atom + 1-Pentene							
82 BIE/HAR Photoionization Mass-spectrometry. Discharge-flow. P(Total) ~ 2 torr.	EX	298	(2.83±0.30)(12)			2	
O + (CH ₃) ₂ CHCH=CH ₂ → products							
Oxygen atom + 1-Butene, 3-methyl-							
74 MCC k _{ref} : O + (CH ₃) ₂ C=CH ₂ → products.	RL	298	(2.2±0.5)(-1)			2/2	1.2
76 SIN/CVE	EX	298-480	(6.02±0.44)(12)	0	266±26	2	
O + (CH ₃) ₂ C=CHCH ₃ → products							
Oxygen atom + 2-Butene, 2-methyl-							
74 FUR/ATK	EX	298	(3.11±0.30)(13)			2	
78 ATK/PIT2 NO ₂ chemiluminescence. Flash-photolysis.	EX	299-441	1.51(13)	0	-191±101	2	
80 SUG/ISH1 Resonance-absorption. Pulse-radiolysis. P = (50-950) torr.	EX	296	(3.31±0.30)(13)			2	
O(¹ D) + (CH ₃) ₂ C=CHCH ₃ → products							
Oxygen atom + 2-Butene, 2-methyl-							
79 KAJ/FUE N ₂ O photolysis. Gas-chromatography. P(Total) = 200 torr. k _{ref} : O(¹ D) + N ₂ O → N ₂ + O ₂	RL	298	(8.9±2.0)			2/2	
O +  → products							
Oxygen atom + Cyclopentane							
72 HUI/HER3 Discharge-flow. Mass-spectrometry.	EX	337-652	1.26(14)	0	2210±100	2	1.23

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O + (CH_3)_3CCH_2 \rightarrow H + (CH_3)_3CCHO$ (a) $\rightarrow HCHO + (CH_3)_3C$ (b) Oxygen atom + Propyl, 2,2-dimethyl-						
79 HOY/SIE1 $k_a + k_b$. Low pressure nozzle reactor. Mass-spectrometry. P = (0.01-0.2) torr.	RN	300	3.3(13)			2
$O(^1D) + CH_3CH_2CH_2CH_2CH_3 \rightarrow$ products Oxygen atom + Pentane						
74 MIC/PAR $k_{ref}: O(^1D) + (CH_3)_4C \rightarrow$ products.	RL	300	(9.88±0.32)(-1)			2/2
$O + (CH_3)_4C \rightarrow OH + (CH_3)_3CCH_2$ Oxygen atom + Propane, 2,2-dimethyl- (Neopentane)						
82 MIC/KEI Reaction of O atoms with Neopentane in Ar/N ₂ buffer gas. Discharge-flow. Resonance-fluorescence. O atoms generated by the photodecomposition of O ₂ . P(Neopentane) = (44.3-215) mtorr. P(Total) = (30-100) torr. P(O ₂) = (0.40-6.0) torr.	EX	415-922	(9.15±1.69)(13)	0	3595±99	2
$O(^1D) + (CH_3)_4C \rightarrow$ products Oxygen atom + Propane, 2,2-dimethyl- (Neopentane)						
71 SCO/CVE $k_{ref}: O(^1D) + N_2O \rightarrow O_2 + N_2$ (a) $\rightarrow NO + NO$ (b)	RL	296	(4.29±0.25)			2/2
75 GAU/SNE $k_{ref}: O(^1D) + O_2 \rightarrow O + O_2(^1\Sigma_g^+)$	RL	300	(1.4±0.2)(1)			2/2
75 GAU/SNE	RN	300	6.26(14)			2
76 FLE/HUS	EX	300	(7.41±0.78)(14)			2
$O + CH_3CH_2CH_2CH_2CH_2SH \rightarrow OOH + CH_3CH_2CH_2CH_2CH_2S$ Oxygen atom + 1-Pentanethiol (Pentyl mercaptan)						
78 KIR/VET Initial step in a suggested mechanism. Supersonic molecular beam. Fast flow-reactor. Mass-spectrometry.	EX	302-409	(6.18±0.35)(12)	0	328±19	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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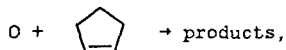


Oxygen atom + 1,3-Cyclohexadiene

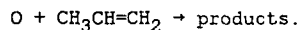
75 GAF/ATK2 ¹⁾	RN	296-423	5.1(12)	0	-664±91	2
75 GAF/ATK2 ¹⁾	RN	296	(5.03±0.23)(13)			2

¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N₂O. Gas-chromatography.

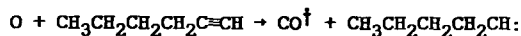
k determined relative to the reaction:



and placed on an absolute basis by using the k expression from the literature, for the reaction:



Supersedes 75 GAF/ATK1.



Oxygen atom + 1-Hexyne

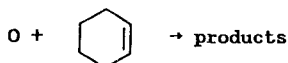
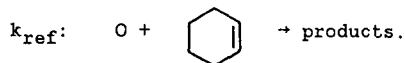
80 SHA/BUR	EX	293	(3.6±0.4)(11)			2
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Flash-photolysis. CO laser Resonance-absorption.



Oxygen atom + 2,3-pentadiene, 2-methyl-

74 HAV	RL	298	3.03			2/2
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Oxygen atom + Cyclohexene

82 WAS/TAK	EX	298	(1.20±0.03)(13)			2
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Reaction of Cyclohexene with O atoms in a fast flow-reactor.

O atoms generated by a microwave-discharge in a He/O₂ mixture.





Mass-spectrometry.

P(Cyclohexene) = (0.004-0.012) mtorr.

[O₂]₀ = (0.266-0.560) mtorr.

P(Total) = 3.7 torr.


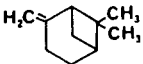

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O + (CH₃)₂C=C(CH₃)₂ → products						
Oxygen atom + 2-Butene, 2,3-dimethyl-						
74 FUR/ATK	EX	298	(4.44±0.41)(13)			2
73 DAV/HUI	EX	298-355	(3.36±0.64)(12)	0	-790±60	2
75 SIN/FUR	EX	298-481	(1.24±0.12)(13)	0	-390±38	2
O +  → OH + 						
Oxygen atom + Cyclohexane → Hydroxyl + Cyclohexyl						
75 KIM/TIM	EX	344-513	(3.2±0.6)(14)	0	2214±201	2
Reaction of Oxygen atom with Cyclohexane in an ESR-flow apparatus. Mass-spectrometry. [Cyclohexane] = (1.8-6.0)10 ¹³ molec.cm ⁻³ . P = (0.33-0.94) torr.						
82 WAS/TAK	EX	298	(5.84±0.36)(10)			2
Reaction of Cyclohexane with O atoms in a fast-flow reactor. O atoms generated by a microwave-discharge in a He/O ₂ mixture. Mass-spectrometry. P(Cyclohexane) = (0.010-0.028) mtorr. P(Total) = (3.8-3.9) torr. [O ₂] ₀ = (13.7-16.1) mtorr.						
72 HUI/HER3	EX	337-652	2.23(14)	0	2350±100	2 1.23
k _p . Discharge-flow. Mass-spectrometry.						
O +  → products						
Oxygen atom + Cyclohexene, 1-methyl-						
75 GAF/ATK2 ¹⁾	RN	296-423	5.3(12)	0	-669±111	2
75 GAF/ATK2 ¹⁾	RN	296	(4.89±0.20)(13)			2
¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. Gas-chromatography. k determined relative to the reaction:						
O +  → products,						
and placed on an absolute basis by using the k expression from the literature, for the reaction:						
O + CH ₃ CH=CH ₂ → products.						
Supersedes 75 GAF/ATK1.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
<p>O +  → products</p> <p>Oxygen atom + Cycloheptane</p> <p>72 HUI/HER3</p> <p>Discharge-flow. Mass-spectrometry.</p>	EX	337-652	2.88(14)	0	2230±100	2 1.3
<p>O(¹D) + (CH₃)₃CCH₂CH(CH₃)₂ → products</p> <p>Oxygen atom + Pentane, 2,2,4-trimethyl-</p> <p>74 MIC/PAR</p> <p>k_{ref}: O(¹D) + (CH₃)₄C → products.</p>	RL	300	(1.257±0.041)			2/2
<p>O +  → products</p> <p>Oxygen atom + Cyclohexene, 1-methyl- 4-(1-methylethenyl)-, (R)- (d-Limonene, or (+)-Limonene)</p> <p>75 GAF/ATK2 ¹⁾</p> <p>75 GAF/ATK2 ¹⁾</p>	RN	296-423	1.1(14)	0	151±75	2
	RN	296	(6.50±0.53)(13)			2
<p>¹⁾ Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N₂O. Gas-chromatography. k determined relative to the reaction:</p> <p>O +  → products,</p> <p>and placed on an absolute basis by using the k expression from the literature, for the reaction: O + CH₃CH=CH₂ → products. Supersedes 75 GAF/ATK1.</p>						
<p>O +  → products</p> <p>Oxygen atom + Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- (α-Pinene)</p> <p>75 GAF/ATK2 ¹⁾</p>	RN	296-423	7.5(13)	0	458±70	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 GAF/ATK2 ¹⁾ 1) Competitive technique. Static system. O-atoms generated by Hg-photosensitized dissociation of N ₂ O. k determined relative to the reaction: O +  → products, and placed on an absolute basis by using the k expression from the literature, for the reaction: O + CH ₃ CH=CH ₂ → products. Supersedes 75 GAF/ATK1.	RN	296	(1.60±0.06)(13)			2
O +  → products Oxygen atom + Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- (β-Pinene)						
75 GAF/ATK2 ¹⁾	RN	296-423	6.0(13)	0	413±70	2
75 GAF/ATK2 ¹⁾	RN	296	(1.51±0.06)(13)			2
1) Competitive technique. Static system. O atoms generated by Hg-photosensitized dissociation of N ₂ O. k determined relative to the reaction: O +  → products, and placed on an absolute basis by using the k expression from the literature, for the reaction: O + CH ₃ CH=CH ₂ → products. Supersedes 75 GAF/ATK1.						
O₂ (+ M) → O + O (+ M) Oxygen molecule						
71 BRE/BIR M = Kr. M-efficiencies relative to Kr are: 1.0(Kr), ~1.6(Xe), ~1.0(Ar), ~9.0(O ₂).	EX	4000-8500	7.87(13)	0	52743	2
O₂(¹A_g) + O₃ → O₂ + O₂ + O Oxygen molecule + Ozone						
71 FIN/SNE	EX	283-321	2.74(13)	0	2828±181	2
72 BEC/GRO	EX	296-360	3.61(13)	0	2854±143	2
72 HUS/KIR1 Upper-limit k.	EX	300	<6.02(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
73 COL/HUS	EX	300	(2.65±0.78)(9)			2	
74 SNE	EX	298	(1.39±0.30)(13)			2	
80 ARN/COM UV-photolysis of Ozone.	EX	298	(3.07±0.30)(9)			2	
74 KUR/BRA $k_{ref}: O_2(^1\Delta_g) + O_3^\dagger \rightarrow O_2 + O_2 + O$ O_3^\dagger formed by absorption of CO ₂ laser radiation.	RL	300	(2.63±0.91)(-2)			2/2	
$O_2(^1\Sigma_g^+) + O_3 \rightarrow O_2 + O_2 + O$ (a) $\rightarrow O_2 + O_3$ (b)							
Oxygen molecule + Ozone							
82 OGR/SWO $k_a + k_b$. Flash-photolysis of O ₂ /O ₃ mixtures in a vacuum system. P(Total) = 100 torr.	EX	298	(1.1±0.2)(13)			2	
$O_2^\dagger + O_3 \rightarrow O + O_2 + O_2$							
Oxygen molecule + Ozone							
80 ARN/COM UV-photolysis of Ozone. O ₂ is vibrationally excited, with $v \leq 30$.	EX	298	(1.69±0.18)(9)			2	
$O_2 + H_2 \rightarrow OH + OH$ (a) $\rightarrow HO_2 + H$ (b)							
Oxygen molecule + Hydrogen molecule							
71 BEL/BRA k_a . Constant tube-area.	ES	1128-1152	2.10(12)	0	19628	2	
71 BEL/BRA k_a . Varying tube-area.	ES	1128-1152	1.20(12)	0	19628	2	
71 JAC/HOU k_a . Reaction behind incident shock-waves, in Ar. UV-Absorption-spectroscopy.	EX	1200-1800	1.7(13)	0	24233	2	3.0
75 AZA/ALE k_a .	EX	1076-1523	1.90(4)	0	21892±503	2	1.58
72 SKI/LIF k_b .	ES	1000-2500	3.0(13)	0	31706	2	
79 HAC/PRE1 k_b . Isothermal flow-reactor. Laser Magnetic Resonance Spectrometry. P(Total) = (130-800) Pa.	DE	298	2.9(-29)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O₂ + D₂ → OD + OD							
Oxygen molecule + Deuterium molecule							
75 AZA/ALE	EX	843	(1.02±0.24)(3)			2	
75 AZA/ALE	EX	843	(7.83±3.01)(2)			2	
k based on induction period.							
O₂(¹Δ_g) + SO₂ → O + SO₃							
Oxygen molecule + Sulfur dioxide							
76 DUM	EX	298	1.3(8)			2	
O₂ + CO₂[*] → O₃ + CO							
Oxygen molecule + Carbon dioxide							
71 PRA/MAK	RL	293	(5.0±2.0)(2)			2/2	
M = CO.							
Photolysis of O ₂ + CO mixture.							
P(CO) = (1-60) torr.							
P(O ₂) = 40 torr.							
k _{ref} : CO ₂ [*] + M → CO ₂ ^{**} + M.							
CO [*] formed by O(¹ D) + CO.							
O₂ + CH₄ → HO₂ + CH₃							
Oxygen molecule + Methane							
72 SKI/LIF	ES	1000-2500	8.00(13)	0	28183	2	
78 SHA	DE	300-2500	7.56(11)	2.0	26153	2	
The preexponential factor expressed as: A(T/298) ² .							
82 PAR	EX	1097	<9.53(5)			2	
Reaction of CH ₄ with O ₂ in single-pulse shock-waves.							
Mass-spectrometry.							
Upper-limit k.							
O₂ + HCHO → HO₂ + CHO							
Oxygen molecule + Formaldehyde							
71 BAL/LAN	RN	713	1.3(1)			2	
74 BAL/FUL2	EX	713-816	2.04(13)	0	19577±755	2	
O₂ + HCHO[*] [or HC(:)OH] → [HC(:)OH.O₂]							
Oxygen molecule + Formaldehyde (or Methylene, hydroxy-)							
79 MOR/HEI	RL	296	(7.9±0.6)(6)			2/1	
HCHO photolysis at 313 nm.							
k _{ref} :							
HCHO [*] [or HC(:)OH] → H + CHO							


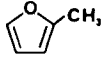
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$O_2 + CH_3O_2NO + CH_3O_2NO \rightarrow CH_3ONO_2 + CH_3ONO_2 + O_2$ Oxygen molecule + Peroxynitrous acid methyl ester	ES	298	$\approx 3.79(13)$			3
73 SPI/VIL Determined on the basis of a suggested mechanism.						
$O_2 + C_2O \rightarrow CO_2 + CO$ Oxygen molecule + Carbon oxide (C_2O)	EX	298	$(1.99 \pm 0.07)(11)$			2
80 DON/PIT Laser photodissociation of C_3O_2 at 266 nm. Dye-laser induced fluorescence.						
$O_2(a^1\Delta_g) + CH \equiv CH \rightarrow \text{products}$ Oxygen molecule + Ethyne	EX	298	$(1.03 \pm 0.08)(7)$			2
79 DAT/RAO Microwave discharge-flow system.						
$O_2 + CH_3CHO (+ M) \rightarrow HO_2 + CH_3CO (+ M)$ Oxygen molecule + Acetaldehyde	RN	336	6.8(-3)			2
74 DIX/SKI1 ¹⁾						
74 DIX/SKI1 ¹⁾	RN	345	7.4(-3)			2
74 DIX/SKI1 ¹⁾	RN	393	6.15(-2)			2
¹⁾ Surface/volume ratio = 0.6 cm^{-1} .						
74 DIX/SKI1 ²⁾	RN	345	2.9(-2)			2
74 DIX/SKI1 ²⁾	RN	393	5.1(-1)			2
¹⁾ Surface/volume ratio = 6.1 cm^{-1} .						
77 COL/NAE The preexponential factor expressed as: $A(T/298)^{0.5}$.	ES	1030-1115	3.45(14)	0.5	21238±604	2 2.0
76 BRY/LEV M = O_3 .	EX	393-473	5.01(17)	0	7549±856	3 7.08
$O_2 + CH_3CH_2CHO \rightarrow HO_2 + CH_3CH_2CO$ Oxygen molecule + Propanal	RN	713	7.6(1)			2
71 BAL/LAN						
74 DIX/SKI1	RN	337	3.4(-2)			2
79 BAL/LEW1 Oxidation in an aged boric-acid-coated vessel.	EX	713	$(8.1 \pm 1.5)(1)$			2
$O_2(a^1\Delta_g) + (CH_3)_2CO \rightarrow \text{products}$ Oxygen molecule + 2-Propanone	EX	298	$(5.9 \pm 0.8)(6)$			2
79 DAT/RAO Microwave discharge flow system.						





4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_2(a^1\Delta_g) + CH_3CH_2CH=CH_2 \rightarrow$ products							
Oxygen molecule + 1-Butene							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.11±0.05)(7)			2	
$O_2(a^1\Delta_g) + cis-CH_3CH=CHCH_3 \rightarrow$ products							
Oxygen molecule + 2-Butene, (Z)-							
75 ASH/OGR	EX	300-500	1.26(11)	0	3256±141	2	1.38
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.42±0.05)(7)			2	
$O_2(a^1\Delta_g) + trans-CH_3CH=CHCH_3 \rightarrow$ products							
Oxygen molecule + 2-Butene, (E)-							
75 ASH/OGR	EX	300-500	1.518(11)	0	3664±181	2	1.51
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.50±0.07)(7)			2	
$O_2(a^1\Delta_g) + (CH_3)_2C=CH_2 \rightarrow$ products							
Oxygen molecule + 1-Propene, 2-methyl-							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(2.02±0.02)(7)			2	
$O_2(a^1\Delta_g) + CH_3CH_2CH_2CH_3 \rightarrow$ products							
Oxygen molecule + Butane							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.05±0.40)(6)			2	
$O_2(a^1\Delta_g) + CH_3C(O)OCH=CH_2 \rightarrow$ products							
Oxygen molecule + Acetic acid ethenyl ester (Vinyl acetate)							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(8.2±0.9)(6)			2	
$O_2(a^1\Delta_g) + CH_2=CHC(O)OCH_3 \rightarrow$ products							
Oxygen molecule + 2-Propenoic acid methyl ester							
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.27±0.02)(7)			2	
$O_2 + (CH_3)_2CHCHO \rightarrow HO_2 + (CH_3)_2CHCO$							
Oxygen molecule + Propanal, 2-methyl-							
79 BAL/CLE Aged boric-acid-coated vessel. P(Total) = 60 torr.	EX	713	(1.2±0.1)(2)			2	





4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_2(a^1\Delta_g) + CH_3C(O)OCH_2CH_3 \rightarrow$ products							
Oxygen molecule + Acetic acid ethyl ester (Ethyl acetate)							
79 DAT/RAO Microwave discharge flow system.	EX	298	(6.3±0.1)(6)			2	
$O_2(^1\Delta_g) +$  \rightarrow products							
Oxygen molecule + Cyclopentene							
75 ASH/OGR	EX	300-500	2.24(11)	0	3719±357	2	2.29
$O_2(^1\Delta_g) + CH_3CH=C(CH_3)_2 \rightarrow$ products							
Oxygen molecule + 2-Butene, 2-methyl-							
73 HUI/HER	RL	298	4.4(-2)			2/2	
k_{ref} :							
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.							
73 HUI/HER	RN	298	3.3(7)			2	
75 ASH/OGR	EX	300-500	1.26(11)	0	2466±141	2	1.45
$O_2 + (CH_3)_2CHCH_2CH_3 \rightarrow HO_2 + (CH_3)_2CCH_2CH_3$ (a)							
$\rightarrow HO_2 + (CH_3)_2CHCH_2CH_3$ (b)							
Oxygen molecule + Butane, 2-methyl- (Isopentane)							
73 DEG/DEN $k_a + k_b$.	EX	410-439	1.5(15)	0	19124	2	
$O_2(^1\Delta_g) +$  \rightarrow products							
Oxygen molecule + Furan, 2-methyl-							
73 HUI/HER	RL	298	1.3			2/2	
k_{ref} :							
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.							
73 HUI/HER	RN	298	1.0(8)			2	
$O_2(a^1\Delta_g) + CH_2=CHC(O)OCH_2CH_3 \rightarrow$ products							
Oxygen molecule + 2-Propenoic acid ethyl ester							
79 DAT/RAO Microwave discharge flow system.	EX	298	(1.54±0.11)(7)			2	

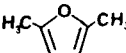


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O_2(^1\Delta_g) + CH_2=C(CH_3)C(O)OCH_3 \rightarrow$ products Oxygen molecule + 2-Propenoic acid, 2-methyl-, methyl ester						
79 DAT/RAO Microwave discharge flow system.	EX	298	(1.09±0.09)(7)			2
$O_2(^1\Delta_g) +$  \rightarrow products						
Oxygen molecule + 1,3-Cyclohexadiene						
73 HUI/HER k_{ref} : $O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.	RL	298	9.0(-2)			2/2
73 HUI/HER	RN	298	6.8(7)			2
$O_2(a^1\Delta_g) +$  \rightarrow products						
Oxygen molecule + 1,4-Cyclohexadiene						
79 DAT/RAO Microwave discharge-flow system.	EX	298	(1.36±0.06)(7)			2
$O_2(^1\Delta_g) +$  \rightarrow products						
Oxygen molecule + Cyclohexene						
75 ASH/OGR Lower-limit estimate.	ES	300-500	2.51(11)	0	>4127	2
79 DAT/RAO Microwave discharge-flow system.	EX	298	(4.7±1.5)(6)			2
$O_2(^1\Delta_g) +$  \rightarrow products						
Oxygen molecule + Cyclopentene, 1-methyl-						
73 HUI/HER k_{ref} : $O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.	RL	298	1.5(-1)			2/2
73 HUI/HER	RN	298	1.1(7)			2
75 ASH/OGR	EX	300-500	2.51(11)	0	3010±141	2 1.45


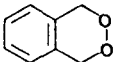
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_2(^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Cyclobutene, 1,2-dimethyl-							
75 ASH/OGR	EX	300-500	2.75(11)	0	2011±91	2	1.29
$O_2(^1\Delta_g) + \text{trans-CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CHCH}_3 \rightarrow \text{products}$							
Oxygen molecule + 2-Pentene, 3-methyl-, (E)-							
73 HUI/HER	RL	298	~1.2(-2)			2/2	
Estimated ratio.							
$k_{\text{ref}}: O_2(^1\Delta_g) + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products.}$							
73 HUI/HER	ES	298	~9.0(6)			2	
$O_2(^1\Delta_g) + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}$							
Oxygen molecule + 2-Butene, 2,3-dimethyl-							
72 ACK/PIT	EX	298	(4.9±0.3)(8)			2	
P > 3 torr.							
73 HUI/HER	EX	298	7.6(8)			2	
75 ASH/OGR	EX	300-500	1.32(11)	0	1626±75	2	1.23
76 DUM	EX	298	2.0(7)			2	
$O_2 + $  $ \rightarrow \text{HO}_2 + $ 							
Oxygen molecule + Cyclohexane							
75 SHA/DEN	EX	373-413	1.58(110)	0	12562±805	2	
$O_2(a^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Cyclohexane							
79 DAT/RAO	EX	298	(1.08±0.30)(6)			2	
Microwave discharge-flow system.							
$O_2(a^1\Delta_g) + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{products}$							
Oxygen molecule + Hexane							
79 DAT/RAO	EX	298	(9.2±3.0)(5)			2	
Microwave discharge flow system.							

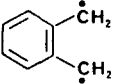
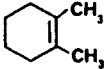
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$O_2(^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Furan, 2,5-dimethyl-							
73 HUI/HER	RL	298	1.9(1)				2/2
$k_{\text{ref}}: O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products}.$							
73 HUI/HER	RN	298	1.5(10)				2
$O_2(a^1\Delta_g) + (CH_3)_2CHCH_2OCH=CH_2 \rightarrow \text{products}$							
Oxygen molecule + Propane, 1-(ethenyloxy)-2-methyl-							
79 DAT/RAO	EX	298	(1.17±0.12)(7)				2
Microwave discharge-flow system.							
$O_2(a^1\Delta_g) + CH_3C(O)CH_2CH(CH_3)_2 \rightarrow \text{products}$							
Oxygen molecule + 2-Pentanone, 4-methyl-							
79 DAT/RAO	EX	298	(4.9±0.9)(6)				2
Microwave discharge-flow system.							
$O_2(^1\Delta_g) + (CH_3)_2C=CHN(CH_3)_2 \rightarrow \text{products}$							
Oxygen molecule + 1-Propen-1-amine, N,N,2-trimethyl-							
73 HUI/HER	RL	298	2.0(1)				2/2
$k_{\text{ref}}: O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products}.$							
73 HUI/HER	RN	298	1.5(10)				2
$O_2(^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Cyclohexene, 1-methyl-							
75 ASH/OGF	EX	300-500	2.40(11)	0	3785±151	2	1.41
$O_2(^1\Delta_g) + $  $ \rightarrow \text{products}$							
Oxygen molecule + Cyclopentene, 1,2-dimethyl-							
73 HUI/HER	RL	298	4.0(-1)				2/2
$k_{\text{ref}}: O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products}.$							
73 HUI/HER	RN	298	3.0(8)				2
75 ASH/OGF	EX	300-500	3.16(11)	0	2023±141	2	1.45

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A k err. units factor
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)CH_2CH_3 \rightarrow$ products						
Oxygen molecule + 2-Pentene, 2,3-dimethyl-						
73 HUI/HER	RL	298	6.9(-1)			2/2
$k_{ref}: O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow$ products.						
73 HUI/HER	RN	298	5.2(8)			2
$O_2 + CH_3(CH_2)_5CH_3 \rightarrow HO_2 + CH_3(CH_2)_5CH_2$ (a)						
$\rightarrow HO_2 + CH_3(CH_2)_4CHCH_3$ (b)						
$\rightarrow HO_2 + CH_3(CH_2)_3CHCH_2CH_3$ (c)						
$\rightarrow HO_2 + CH_3(CH_2)_2CH(CH_2)_2CH_3$ (d)						
Oxygen molecule + Heptane						
75 SHA/DEN	EX	397-434	3.16(17)	0	21792±2013	2
$k_a + k_b + k_c + k_d$.						
$O_2(a^1\Delta_g) + CH_2=CHCOOCH_2CH_2CH_2CH_3 \rightarrow$ products						
Oxygen molecule + 2-Propenoic acid butyl ester						
79 DAT/RAO	EX	298	(1.36±0.08)(7)			2
Microwave discharge-flow system.						
$O_2(a^1\Delta_g) + CH_3(CH_2)_5CHO \rightarrow$ products						
Oxygen molecule + Heptanal						
79 DAT/RAO	EX	298	(6.9±0.1)(6)			2
Microwave discharge-flow system.						
$O_2(a^1\Delta_g) + CH_3COOCH_2CH_2CH(CH_3)_2 \rightarrow$ products						
Oxygen molecule + 1-Butanol, 3-methyl-, acetate						
79 DAT/RAO	EX	298	(5.2±1.1)(6)			2
Microwave discharge-flow system.						
$O_2 +$		\rightarrow				
Oxygen molecule + 1,3-Cyclohexadiene, 5,6-bis(methylene)-						
\rightarrow 2,3-Benzodioxin, 1,4-dihydro-						
82 ROT/SCH1	EX	461-521	(1.9±1.2)(10)	0	5687±301	2
Thermal reaction in an air thermostat.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
5,6-bis(Methylene)-1,3-cyclohexadiene is in equilibrium with its intermediate form, the biradical						
						
(1,2-Phenylenebismethyl) before reacting with O ₂ .						
$O_2(^1\Delta_g) + $  $ \rightarrow \text{products}$						
Oxygen molecule + Cyclohexene, 1,2-dimethyl-	73 HUI/HER	RL	298	4.0(-1)		2/2
k_{ref} :						
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products.}$	73 HUI/HER	RN	298	3.0(8)		2
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)CH_2CH_2CH_3 \rightarrow \text{products}$						
Oxygen molecule + 2-Hexene, 2,3-dimethyl	73 HUI/HER	RL	298	6.6(-1)		2/2
k_{ref} :						
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products.}$	73 HUI/HER	RN	298	5.0(8)		2
$O_2 + (CH_3)_3CCH_2CH(CH_3)_2 \rightarrow HO_2 + (CH_3)_3CCH_2C(CH_3)_2$ (a)						
$\rightarrow HO_2 + (CH_3)_3CCHCH(CH_3)_2$ (b)						
Oxygen molecule + Pentane, 2,2,4-trimethyl-	73 DEG/DEN	EX	400-465	1.0(15)	0 19124	2
$k_a + k_b$.						
$O_2(^1\Delta_g) + CH_3CH_2OCH=C(CH_2CH_3)CH_2CH_2CH_2CH_3 \rightarrow \text{products}$						
Oxygen molecule + 1-Hexene, 1-ethoxy-2-ethyl-	73 HUI/HER	RL	298	~5.0(-1)		2/2
Estimated ratio.						
k_{ref} :						
$O_2(^1\Delta_g) + (CH_3)_2C=C(CH_3)_2 \rightarrow \text{products.}$	73 HUI/HER	RN	298	~4.0(8)		2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O₃ (+ M) → O₂ + O (+ M)							
Ozone							
79 END/GLA M = N ₂ . M-efficiencies relative to N ₂ are: 1.29(He), 0.79(Ne), 0.46(Ar), 0.66(Kr), 0.51(Xe), 1.00(N ₂), 0.94(O ₂), 3.86(CO ₂), 2.43(CF ₄), 6.43(SF ₆). Thermal dissociation in shock-waves. Rate constants expressed as k[M].	EX	800	3.5(8)			2	
79 HEI/COF M = O ₃ . Critical evaluation.	EX	300-3000	4.32(14)	0	11173	2	
80 KLA/LAU M = O ₂ (a ¹ Δ _g , v>1). Flash-photolysis of Ozone. Absorption-Spectroscopy. Resonance-fluorescence. Upper-limit k.	EX	298	≤3.01(11)			2	
80 TOB/ULL M = CO ₂ . Vacuum system. P < 1.0x10 ⁻⁵ torr.	EX	348-433	2.00(15)	0	11726±705	2	7.94
82 EGO/POP M = O ₃ . Thermolysis of O ₃ in a static system. P = (75-100) torr.	EX	423	1.87(3)			2	
O₃ + SO → O₂ + SO₂							
Ozone + Sulfur monoxide							
80 ROB/SMI Pulsed laser photolysis of O ₃ in excess N ₂ and in presence of COS. P(Total) = 100 torr.	EX	296	(5.24±0.96)(10)			2	
82 BLA/SHA1 ¹⁾	EX	298	(6.38±0.96)(10)			2	
82 BLA/SHA2 ¹⁾	EX	230-420	2.89(13)	0	1170±120	2	1.33
¹⁾ SO generated by ArF laser-photodissociation of SO ₂ at 193 nm. in He diluent. P(SO ₂) ~ 30 mtorr. P(O ₂) < 550 torr. P(O ₃) < 0.4 torr. P(He) = 200 torr.							
O₃(v=n) + SO → O₂ + SO₂(¹B₁)							
Ozone + Sulfur monoxide							
74 KAL/BRA O ₃ [†] produced by CO ₂ laser radiation. k _{ref} : O ₃ + SO → O ₂ + SO ₂ (¹ B ₁).	RL	300	(2.4±0.6)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O₃ + SO₂ → O₂ + SO₃							
Ozone + Sulfur dioxide							
74 DAV/PRU Upper-limit k.	EX	300	≤6.02(1)			2	
O₃ + H₂S → HO₂ + HSO (a) → OH + HSO₂ (b)							
Ozone + Hydrogen sulfide							
75 BEC/INO k _a + k _b . Upper-limit k. Unreported T assumed to be 298 K.	EX	298	<1.20(4)			2	
75 GLA/TOB1 k _a = k _b .	ES	298	5.0(5)			2	
75 GLA/TOB1 k _a + k _b .	ES	293-343	1.26(11)	0	3422±302	2	2.51
75 GLA/TOB2 k _a + k _b .	EX	298-343	1.58(12)	0	2617±604	2	6.31
O₃ + NO → O₂ + NO₂(²A₁) (a) → O₂ + NO₂[†](²A₁) (b) → O₂ + NO₂[*](²B_{1,2}) (c)							
O₃ + NO[†] → O₂ + NO₂(²A₁) (d) → O₂ + NO₂[*](²B_{1,2}) (e)							
O₃[†] + NO → O₂ + NO₂(²A₁) (f) → O₂ + NO₂[†](²A₁) (g) → O₂ + NO₂[*](²B_{1,2}) (h) → O₃ + NO (i)							
Ozone + Nitrogen oxide (NO)							
73 GHO/ELL k _a .	EX	298	(8.5±0.1)(9)			2	
73 STE/NIK1 k _a .	EX	298	(1.04±0.06)(10)			2	
74 BEC/SCH k _a .	EX	290	1.02(10)			2	
74 BEM/CLY k _a .	EX	298	(1.09±0.08)(10)			2	
75 HUI/HER2 k _a . Tubular flow reactor. Mass-spectrometer.	EX	224-364	(2.09±0.24)(12)	0	1533±32	2	
75 WU/NIK k _a . NO ₂ Photolysis.	EX	298	1.11(10)			2	
76 BIR/SHO k _a .	EX	203-361	(1.41±0.14)(12)	0	1450±50	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 FRE/STE $k_a + k_c + k_f + k_h$. $O_3^\dagger = O_3(001)$ (asymmetric stretch.)	EX	298	(1.46±0.15)(11)			2
76 STE/FRE $(k_a + k_c + k_f)/k_a$. Upper-limit ratio.	RL	298	≤2.2(1)			2/2
80 LIP/JES k_a . Stainless-steel reactor. P < 0.1 mtorr.	EX	283-443	(2.59±0.36)(12)	0	1598±50	2
81 MIC/ALL k_a . Fast-flow. Induced fluorescence detection of [NO].	EX	195-369	(1.57±0.48)(12)	0	1435±64	2
81 RAY/WAT ¹⁾	EX	212-422	(1.90±0.54)(12)	0	1556±80	2
81 RAY/WAT ¹⁾	EX	299	(1.08±0.05)(10)			2
¹⁾ k_a . Discharge-flow Mass-Spectrometry. $[O_3]_0 = (0.05-1.82) \times 10^{12}$ molec.cm ⁻³ $[NO]_0 = (0.07-1.94) \times 10^{16}$ molec.cm ⁻³						
81 SCH/LIP k_a . Spherical reactor. (7-120) × 10 ⁻⁶ torr.	EX	283-433	(1.37±0.24)(12)	0	1475±62	2
82 BOR/BIR ²⁾ Preexponential factor expressed as: $A(T/298)^{2.2}$.	EX	200-350	(1.49±0.15)(11)	2.2	765±116	2
82 BOR/BIR ²⁾ ²⁾ k_a . Reaction of NO with O ₃ in He, by using a dual flow-tube technique. Mass-spectrometry. $[O_3] = (0.05-1.00) \times 10^{13}$ molec.cm ⁻³ . $[NO] = (0.5-6.0) \times 10^{15}$ molec.cm ⁻³ .	EX	298	(1.14±0.11)(10)			2
81 SCH/LIP k_c . Spherical reactor. (7-120) × 10 ⁻⁶ torr.	EX	283-433	(1.75±0.18)(12)	0	1951±34	2
78 BAR/MOY ³⁾	EX	158	(1.06±0.08)(11)			2
78 BAR/MOY ³⁾	EX	225	(7.5±1.1)(10)			2
78 BAR/MOY ³⁾	EX	296	(9.2±0.4)(10)			2
78 BAR/MOY ³⁾	EX	300	9.9(10)			2
78 BAR/MOY ³⁾	EX	345	(1.24±0.07)(11)			2
78 BAR/MOY ³⁾	EX	437	(1.85±0.16)(11)			2
³⁾ $k_d + k_e + k_i$. O_3^\dagger is either O ₃ (001) (asymmetric stretch), or O ₃ (010) (bending mode), but not both. Other rate constants within the (158-437) K range are given. Non-Arrhenius behaviour. The k is minimum at 225K. Laser-enhanced fluorescence.						
76 STE/FRE k_e/k_c . NO [†] is NO(v=1).	RL	298	5.7			2/2 1.45
76 GOR/LIN k_f . $O_3^\dagger = O_3(001)$ (asymmetric stretch.) Fit of experimental data to a proposed mechanism.	ES	308	(5.4±0.7)(10)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 KUR/BRA k_f . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	ES	153-373	2.23(13)	0	1610	2
75 KUR/BRA k_f . $O_3^\dagger = O_3(001) + O_3(100)$ (asymmetric + symmetric stretch.) Fit of experimental data to a proposed mechanism.	ES	153-373	1.20(13)	0	1107	2
75 KUR/BRA k_f . $O_3^\dagger = O_3(001) + O_3(010) + O_3(100)$. (Sum of all three vibrational modes: asymmetric stretch + bend + symmetric stretch.) Fit of experimental data to a proposed mechanism.	ES	153-373	1.20(13)	0	1525	2
77 MOY/BAR k_f/k_a . $O_3^\dagger = O_3(001)$ (asymmetric stretch.) Pulsed CO_2 laser.	RL	153-303	(8.7±2.1)(-1)	0	-649±55	2/2
73 GOR/LIN k_g . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	ES	350	(1.5±0.2)(11)			2
73 GOR/LIN k_g/k_b . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	RL	350	≈2.2(1)			2/2
74 KUR/BRA k_g/k_c . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	RL	300	(1.71±0.43)(1)			2/2
74 KUR/BRA ($k_g + k_h$)/($k_b + k_c$). $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	RL	300	(1.62±0.40)(1)			2/2
74 KUR/BRA $k_g + k_b$. $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	EX	300	(1.63±0.06)(11)			2
78 HUI/COO2 k_g . $O_3^\dagger = O_3(001) + O_3(010) + O_3(100)$. Sum of all three vibrational modes, of which (001) and (100), - asymmetric and symmetric stretch-, are predominant.) Laser-enhanced fluorescence method.	EX	138-410	(2.29±0.54)(11)	0	518±131	2
76 GOR/LIN k_h . $O_3^\dagger = O_3(001)$ (asymmetric stretch.) Fit of experimental data to a proposed mechanism.	ES	308	(4.3±0.7)(9)			2
74 KUR/BRA k_h/k_c . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	RL	300	(4.1±2.0)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 BRA/KUR k_h/k_c . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism. The authors suggest that the NO_2^* (2B_2) electronic state might very well be the primary emission source, instead of the 2B_1 state.	RL	300	(5.6±1.0)			2/2
77 MOY/BAR k_h/k_c . $O_3^\dagger = O_3(001)$ (asymmetric stretch.)	RL	153-303	(7.6±2.1)			2/2
77 MOY/BAR k_h/k_c . $O_3^\dagger = O_3(001)$ (asymmetric stretch.)	RL	153-303	(8.7±5.5)(-1)	0	-649±126	2/2
78 HUI/COO2 k_h . $O_3^\dagger = O_3(001) + O_3(010) + O_3(100)$. (Sum of all three vibrational modes, of which (001) and (100), - asymmetric and symmetric stretch-, are predominant.) Laser-enhanced fluorescence method.	EX	138-410	(6.02±0.18)(11)	0	1449±211	2
75 KUR/BRA k_i . $O_3^\dagger = O_3(010)$ (bending mode.) Fit of experimental data to a proposed mechanism.	ES	153-373	6.02(10)	0	39.2	2
$O_3 + NO_2 \rightarrow O_2 + NO_3$						
Ozone + Nitrogen oxide (NO_2)						
73 STE/NIK1	EX	298	(3.91±0.48)(7)			2
73 WU/MOR	EX	299	2.65(7)			2 1.15
74 BEC/SCH	EX	289	1.95(7)			2
74 DAV/PRU	EX	260-343	(5.42±0.49)(10)	0	2428±116	2
74 GHO/ELL Corrected rate constant from 73 GHO/ELL.	EX	298	(1.9±0.3)(7)			2
74 GRA/JOH	EX	231-298	(8.07±0.66)(10)	0	2466±30	2
74 HUI/HER	EX	259-362	(9.44±2.46)(10)	0	2509±76	2
75 GRA	EX	231-298	(8.07±0.66)(10)	0	2466±30	2
75 HER/HUI	EX	259-363	(9.44±2.46)(10)	0	2509±76	2
$O_3 + HONO \rightarrow O_2 + HONO_2$						
Ozone + Nitrous acid						
77 KAI/JAP ¹⁾	EX	226	≤3.01(5)			2
77 KAI/JAP ¹⁾	EX	300	≤6.02(4)			2
¹⁾ Upper limit k's. Pyrex reactor in evacuated chamber. P(Total) = (20-30) torr.						
79 STR/WEL Tunable diode-laser. Static reactor. Upper-limit k.	EX	296	≤(2.71±1.81)(5)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O₃ + CH₄ → products							
Ozone + Methane							
73 STE/NIK2 Upper-limit k.	EX	298	≤7.22(2)			2	
O₃ + HCHO → OH + HCO₃ (a) → HO₂ + HCO₂ (b)							
Ozone + Formaldehyde							
76 BRA/HEI k _a + k _b . Upper-limit k.	EX	298	-1.26			2	
O₃ + CH₃ONO → O₂ + CH₃ONO₂							
Ozone + Nitrous acid methyl ester (Methyl nitrite)							
76 HAS/FRE	EX	298-352	4.07(11)	0	5315±172	2	1.70
O₃ + CH=CH → products							
Ozone + Ethyne							
71 DEM	EX	294	(1.8±0.3)(4)			2	
73 STE/NIK2	EX	298	(5.18±0.54)(4)			2	
76 PAT/ATK1	EX	297	(2.29±0.36)(4)			2	
O₃ + CH₂=CH₂ → [C₂H₄.O₃][†] → CH₂OO[†] + HCHO (a) → any other products (b)							
Ozone + Ethene							
80 SU/CAL ¹⁾	EX	298	(1.08±0.06)(6)			2	
81 KAN/SU ¹⁾	EX	282-303	1.55(10)	0	2828±181	2	1.86
¹⁾ k _a . Fourier-transform IR-spectroscopy in O ₂ /N ₂ mixtures. P(Total) = 700 torr. The biradical decomposes further to other products.							
73 STE/WU k _{overall} .	EX	299	(9.34±0.90)(5)			2	
74 BEC/SCH ²⁾	EX	280-360	7.23(9)	0	2491±101	2	
74 BEC/SCH ²⁾	EX	298	1.69(6)			2	
²⁾ k _{overall} .							
74 FIN/PIT k _{overall} . In O ₂ carrier gas.	EX	298	(1.0±1.0)(6)			2	
74 FIN/PIT k _{overall} . In N ₂ carrier gas.	EX	298	(5.0±2.0)(6)			2	
74 HER/HUI k _{overall} .	EX	235-362	(5.42±3.19)(9)	0	2557±167	2	
74 JAP/WU2 k _{overall} .	EX	298	(1.14±0.06)(6)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 JAP/WU k _{overall} . In 760 torr. Air.	EX	299	(1.14±0.06)(6)			2	
76 JAP/WU k _{overall} . In 760 torr. He.	EX	299	(1.56±0.12)(6)			2	
76 TOB/TOB k _{overall} .	EX	303	(1.02±0.08)(6)			2	
76 WIL k _{overall} .	EX	298	8.8(5)			2	
81 ADE/KER ³⁾	EX	260	2.65(5)			2	
81 ADE/KER ³⁾	EX	294	9.64(5)			2	
81 ADE/KER ³⁾ Tentative k.	EX	260-294	~1.9(10)	0	~2919	2	
³⁾ k _{overall} . Reaction carried out in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.							
82 ATK/ASC1 k _{overall} . Reaction of O ₃ with Ethene in a Teflon bag. Gas-chromatography. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³ .	EX	296	(8.61±1.14)(5)			2	
O ₃ + cis-CDH=CDH → [C ₂ D ₂ H ₂ .O ₃] [†] → CDHOO [†] + HCDO Ozone + Ethene-1,2-d ₂ , (Z)-							
80 SU/CAL FTIR Spectroscopy in O ₂ /N ₂ mixtures. The biradical decomposes further to other products. P(Total) = 700 torr.	EX	298	(1.33±0.24)(6)			2	
O ₃ + trans-CDH=CDH → [C ₂ D ₂ H ₂ .O ₃] [†] → CDHOO [†] + HCDO Ozone + Ethene-1,2-d ₂ , (E)-							
80 SU/CAL FTIR Spectroscopy in O ₂ /N ₂ mixtures. The biradical decomposes further to other products. P(Total) = 700 torr.	EX	298	(1.33±0.06)(6)			2	
O ₃ + CD ₂ =CD ₂ → [C ₂ D ₄ .O ₃] [†] → CD ₂ OO [†] + DCDO Ozone + Ethene-d ₄							
74 JAP/WU2	EX	298	(1.38±0.06)(6)			2	
80 SU/CAL FTIR spectroscopy in O ₂ /N ₂ mixtures. The biradical decomposes further to other products. P(Total) = 700 torr.	EX	298	(1.26±0.06)(6)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
O₃ + CH₃CHO → products							
Ozone + Acetaldehyde							
73 STE/NIK2	EX	298	(2.05±0.30)(4)			2	
81 ATK/ASC	EX	296	≤3.61(3)			2	
Reaction in a Teflon bag, in ultra-high purity air. Upper-limit k. P(Total) = 735 torr.							
O₃ + \triangle → CH₂=CH₂ + SO₂							
+ HCHO + CO ₂ (major products)							
Ozone + Thirane (Ethylene episulfide)							
80 MAR/HER	EX	296	<1.0(4)			2	
Stopped-flow autocatalytic reaction. Mass-spectrometry. Upper-limit k. P(Total) = 8 torr.							
O₃ + CH₃CH₂ONO → O₂ + CH₃CH₂ONO₂							
Ozone + Nitrous acid methyl ester							
76 HAS/FRE	EX	298-352	1.90(8)	0	2351±116	2	1.45
O₃ + CH₃C=CH → products							
Ozone + 1-Propyne							
71 DEM	EX	294	(1.3±0.7)(4)			2	
O₃ + CH₂=C=CH₂ → [CH₂=C=CH₂·O₃] → products							
Ozone + 1,2-Propadiene							
74 TOB/TOB	ES	499-598	1.0(9)	0	2768±503	2	5.01
O₃ + CH₃CH=CH₂ → products							
Ozone + 1-Propene							
72 COX/PEN	EX	295	7.6(6)			2	
73 STE/WU	EX	299	(7.53±0.60)(6)			2	
74 BEC/SCH	EX	280-360	6.63(9)	0	1968±101	2	
74 BEC/SCH	EX	298	8.73(6)			2	
74 HER/HUI	EX	235-362	(3.70±1.42)(9)	0	1897±109	2	
74 JAP/WU2	EX	299	(7.82±0.60)(6)			2	
76 JAP/WU	EX	299	(7.95±0.18)(6)			2	
In 760 torr. Air.							
76 JAP/WU	EX	299	(1.01±0.06)(7)			2	
In 760 torr. He.							
76 WIL	EX	298	5.79(6)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 ADE/KER ¹⁾	EX	260	3.07(6)			2
81 ADE/KER ¹⁾	EX	294	7.59(6)			2
81 ADE/KER ¹⁾ Tentative k.	EX	260-294	~7.58(9)	0	~2013	2
¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.						
82 ATK/ASC1 Reaction of O ₃ with 1-Propene in a Teflon bag. Gas-chromatography. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³ .	EX	296	(6.26±0.84)(6)			2
O₃ + CD₃CD=CD₂ → products Ozone + Propene-d ₆						
74 JAP/WU2	EX	298	(9.09±0.18)(6)			2
O₃ + CH₂=CHCHO → products Ozone + 2-Propenal (Acrolein)						
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh-purity air. P(Total) = 735 torr.	EX	296	(1.69±0.30)(5)			2
O₃ + CH₃C(O)CHO → products Ozone + Propanal, 2-oxo-						
76 PAT/ATK1	EX	297	(6.63±3.01)(2)			2
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh-purity air. Upper-limit k. P(Total) = 735 torr.	EX	296	<4.22(4)			2
O₃ + CH₂=CHCN → products Ozone + 2-Propenenitrile (Acrylonitrile)						
82 ATK/ASC1 Reaction of O ₃ with 2-Propenenitrile in a Teflon bag. Gas-chromatography. Upper-limit k. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³ .	EX	296	<6.02(4)			2
O₃ + CH₃CH₂C≡CH → products Ozone + 1-Butyne						
71 DEM	EX	294	(2.4±0.8)(4)			2
O₃ + CH₃C≡CCH₃ → products Ozone + 2-Butyne						
71 DEM	EX	294	(2.0±0.3)(4)			2



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O₃ + CH₂=CHCH=CH₂ → products						
Ozone + 1,3-Butadiene						
74 BEC/SCH	EX	280-360	3.28(10)	0	2682±101	2
74 BEC/SCH	EX	298	4.04(6)			2
74 JAP/WU2	EX	298	(5.06±0.12)(6)			2
75 TOB/TOB	EX	273-343	6.31(10)	0	2919±403	2 3.16
O₃ + CH₃CH₂CH=CH₂ → products						
Ozone + 1-Butene						
74 JAP/WU2	EX	298	(7.41±0.24)(6)			2
75 HUI/HER1	EX	225-363	1.77(9)	0	1686±20	2 1.08
In 0.0015 torr. of O ₂ as scavenger.						
76 WIL	EX	298	5.6(6)			2
81 ADE/KER ¹⁾	EX	260	3.19(6)			2
81 ADE/KER ¹⁾	EX	294	7.59(6)			2
81 ADE/KER ¹⁾	ES	260-294	~6.02(9)	0	~1963	2
¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.						
O₃ + CH₃CH=CHCH₃ → products						
Ozone + 2-Butene						
74 BEC/SCH	EX	280-360	5.66(9)	0	1147±75	2
74 BEC/SCH	EX	298	1.20(8)			2
cis-, and trans-2-Butene mixture.						
O₃ + cis-CH₃CH=CHCH₃ → products						
Ozone + 2-Butene, (Z)-						
72 COX/PEN	EX	295	8.5(7)			2
72 COX/PEN ¹⁾	EX	295	9.0(7)			2
74 FIN/PIT ¹⁾	EX	298	(1.5±0.2)(8)			2
¹⁾ In N ₂ carrier gas.						
74 FIN/PIT	EX	298	(6.3±1.9)(7)			2 1.3
In O ₂ carrier gas.						
74 JAP/WU2	EX	298	(9.70±0.42)(7)			2
75 HUI/HER1	EX	225-336	1.87(9)	0	956±54	2 1.22
In 0.0075 torr. of O ₂ as scavenger.						
76 WIL	EX	298	7.3(6)			2
O₃ + trans-CH₃CH=CHCH₃ → products						
Ozone + 2-Butene, (E)-						
72 COX/PEN	EX	295	1.55(8)			2
73 STE/WU	EX	299	(1.66±0.14)(8)			2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 JAP/WU2	EX	298	(1.57±0.05)(8)			2	
75 HUI/HER1 In 0.0075 torr. of O ₂ as scavenger.	EX	225-363	3.59(9)	0	1051±43	2	1.17
76 JAP/WU In 760 torr. Air.	EX	299	(1.54±0.09)(8)			2	
76 JAP/WU In 760 torr. He.	EX	299	(1.70±0.04)(8)			2	
81 ADE/KER Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.	EX	294	1.73(8)			2	
O₃ + (CH₃)₂C=CH₂ → products							
Ozone + 1-Propene-, 2-methyl-							
74 BEC/SCH	EX	283	1.08(7)			2	
74 FIN/PIT In O ₂ carrier gas.	EX	298	(5.4±2.3)(6)			2	
74 FIN/PIT In N ₂ carrier gas.	EX	298	(3.6±0.6)(7)			2	
75 HUI/HER1 In 0.0075 torr. of O ₂ as scavenger.	EX	225-363	1.91(9)	0	1671±23	2	1.06
74 JAP/WU2	EX	298	(8.19±0.12)(6)			2	
76 WIL	EX	298	7.4(6)			2	
81 ADE/KER Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.	EX	294	7.23(6)			2	
O₃ + CH₃CH=CHCHO → products							
Ozone + 2-Butenal (Crotonaldehyde)							
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh- purity air. P(Total) = 735 torr.	EX	296	(5.42±1.08)(5)			2	
O₃ + CH₃C(O)CH=CH₂ → products							
Ozone + 3-Buten-2-one							
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh- purity air. P(Total) = 735 torr.	EX	296	(2.87±0.36)(6)			2	


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O₃ + CH₂=C(CH₃)CHO → products						
Ozone + 2-Propenal, 2-methyl- (Methacrolein)						
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh-purity air. P(Total) = 735 torr.	EX	296	(6.75±0.78)(5)			2
O₃ +  (+ M) → adduct						
Ozone + Thiophene						
77 KAD/TOB ¹⁾	EX	303-356	6.31(10)	0	4227±352	2 3.16
77 KAD/TOB ¹⁾ M = O ₂ .	EX	303-356	2.51(18)	0	2365±201	3 2.51
¹⁾ High vacuum reaction vessel. P(Thiophene) ≤ 1.0 torr. P(O ₃) ≤ 0.3 torr.						
O₃ + CH₂=C(CH₃)CH=CH₂ → products						
Ozone + 1,3-Butadiene, 2-methyl- (Isoprene)						
81 ADE/KER ¹⁾	EX	260	9.94(6)			2
81 ADE/KER ¹⁾ ¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography. P ~ 760 torr.	EX	294	4.22(6)			2
82 ATK/WIN Reaction in a thermostated environmental chamber. [O ₃] = (4.7-9.5) × 10 ¹² molec.cm ⁻³ .	EX	276-324	9.28(9)	0	2153±430	2
O₃ +  → products						
Ozone + Cyclopentene						
74 JAP/WU2	EX	298	(4.89±0.48)(8)			2
81 ADE/KER ¹⁾	EX	260	3.45(8)			2
81 ADE/KER ¹⁾ ¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. P ~ 760 torr. Gas-chromatography.	EX	294	5.84(8)			2
O₃ + CH₃CH₂CH₂CH=CH₂ → products						
Ozone + 1-Pentene						
74 JAP/WU2	EX	298	(6.44±0.24)(6)			2
O₃ + cis-CH₃CH₂CH=CHCH₃ → products						
Ozone + 2-Pentene, (Z)-						
72 COX/PEN	EX	295	1.26(8)			2

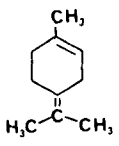
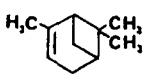
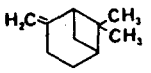
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
O₃ + trans-CH₃CH₂CH=CHCH₃ → products						
Ozone + 2-Pentene, (E)-						
72 COX/PEN	EX	295	1.9(7)			2
O₃ + CH₃CH=C(CH₃)₂ → products						
Ozone + 2-Butene, 2-methyl-						
72 COX/PEN	EX	295	4.8(8)			2
74 JAP/WU2	EX	298	(2.97±0.10)(8)			2
75 HUI/HER1	EX	227-363	3.82(9)	0	826±78	1.32
In 0.0075 torr. of O ₂ as scavenger.						
O₃ + CH₃C(O)CH=CHCH₃ → products						
Ozone + 3-Penten-2-one						
81 ATK/ASC	EX	296	(1.28±0.23)(7)			2
Reaction in a Teflon bag, in ultrahigh-purity air. P(Total) = 735 torr.						
O₃ +  → products						
Ozone + Cyclohexene						
74 JAP/WU1	EX	298	(1.02±0.06)(8)			2
M = Air. Ozonolysis of Cyclohexene in a static reactor. Same data given in 74 JAP/WU2.						
[Cyclohexene] ₀ = (0.51-1.09) × 10 ¹⁴ molec.cm ⁻³ .						
[O ₃] ₀ = (1.22-6.13) × 10 ¹² molec.cm ⁻³ .						
P(Total) = 760 torr.						
81 ADE/KER ¹⁾	EX	260	7.23(8)			2
81 ADE/KER ¹⁾	EX	294	7.11(7)			2
¹⁾ Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography.						
P ~ 760 torr.						
O₃ + CH₃CH₂CH₂CH₂CH=CH₂ → products						
Ozone + 1-Hexene						
72 COX/PEN	EX	295	8.2(6)			2
72 COX/PEN	EX	295	7.2(6)			2
In N ₂ atmosphere.						
73 STE/WU	EX	299	(6.63±0.90)(6)			2
74 JAP/WU2	EX	298	(6.69±0.18)(6)			2
81 ADE/KER	EX	294	6.50(6)			2
Reaction in two Tedlar plastic bags, in synthetic air. Gas-chromatography.						
P ~ 760 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC1 Reaction of O ₃ with 1-Hexene Teflon bag. Gas-chromatography. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³ .	EX	296	(7.29±1.69)(6)			2
O₃ + CH₃CH₂CH₂C(CH₃)=CH₂ → products Ozone + 1-Pentene, 2-methyl-						
72 COX/FEN	EX	295	1.02(7)			2
O₃ + (CH₃)₂CHCH₂CH=CH₂ → products Ozone + 1-Pentene, 4-methyl-						
72 COX/FEN	EX	295	6.4(6)			2
O₃ + cis-CH₃CH₂C(CH₃)=CHCH₃ → products Ozone + 2-Pentene, 3-methyl-, (Z)-						
74 JAP/WU2	EX	298	(2.75±0.48)(8)			2
O₃ + trans-CH₃CH₂C(CH₃)=CHCH₃ → products Ozone + 2-Pentene, 3-methyl-, (E)-						
74 JAP/WU2	EX	298	(3.39±0.10)(8)			2
O₃ + (CH₃)₂C=C(CH₃)₂ → products Ozone + 2-Butene, 2,3-dimethyl-						
74 JAP/WU2	EX	298	(9.09±0.48)(8)			2
75 HUI/HER1 In 0.0075 torr. of O ₂ as scavenger.	EX	227-363	1.70(9)	0	294±196	2 1.73
O₃ +  → products Ozone + 2-Cyclohexen-1-one						
81 ATK/ASC Reaction in a Teflon bag, in ultrahigh-purity air. P(Total) = 735 torr.	EX	296	(7.35±1.57)(5)			2
O₃ + CH₃(CH₂)₄CH=CH₂ → products Ozone + 1-Heptene						
82 ATK/ASC1 Reaction in a Teflon bag. Gas-chromatography. [O ₃] < 2.4x10 ¹³ molec.cm ⁻³	EX	296	(1.04±0.17)(7)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$O_3 + $  $ \rightarrow $ products						
Ozone + Cyclohexene, 1-methyl-4-(1-methylethylidene)- (Terpinolene)						
74 JAP/WU1	EX	296	(4.40±0.66)(8)			2
M = Air. Ozonolysis of Terpinolene in a static reactor.						
P(Total) = 760 torr.						
[Terpinolene] ₀ = (0.39-2.55) × 10 ¹³ molec. cm ⁻³ .						
[O ₃] ₀ = (0.61-1.47) × 10 ¹² molec. cm ⁻³ .						
$O_3 + $  $ \rightarrow $ products						
Ozone + Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- (α-Pinene)						
74 JAP/WU1 ¹⁾	EX	298	(1.99±0.18)(8)			2
M = Air.						
[O ₃] ₀ = (0.61-1.47) × 10 ¹² molec. cm ⁻³ .						
[α-Pinene] ₀ = (0.52-1.32) × 10 ¹³ molec. cm ⁻³ .						
74 JAP/WU1 ¹⁾	EX	298	(2.17±0.18)(8)			2
M = He.						
[α-Pinene] ₀ = (1.05-1.14) × 10 ¹³ molec. cm ⁻³ .						
[O ₃] ₀ = (0.61-1.35) × 10 ¹² molec. cm ⁻³ .						
¹⁾ Ozonolysis of α-Pinene in a static reactor.						
P(Total) = 760 torr.						
82 ATK/WIN	EX	276-324	5.66(8)	0	731±173	2
Reaction in a thermostated environmental chamber.						
Gas-chromatography.						
[O ₃] = (4.7-9.5) × 10 ¹² molec. cm ⁻³ .						
$O_3 + $  $ \rightarrow $ products						
Ozone + Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene- (β-Pinene)						
82 ATK/WIN	EX	296	(1.26±0.30)(7)			2
Reaction in Teflon bag. Gas-chromatography.						
[O ₃] = (4.7-9.5) × 10 ¹² molec. cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A k err. units factor
H + O₂ (+ M) → OH + O (+ M) (a)						
→ HO₂ (+ M) (b)						
Hydrogen atom + Oxygen molecule						
71 BEL/BRA k _a . Constant tube-area.	ES	1128-1152	2.10(14)	0	8354	2
71 BEL/BRA k _a . Varying tube-area.	ES	1128-1152	1.44(14)	0	8354	2
71 BRA/BEL1 k _a .	EX	1150-1400	1.245(14)	0	8203±554	2 1.24
71 BRA/BEL2 k _a . Rankine-Hugoniot measurements in shock-tube at low temperatures.	EX	30-90	1.38(14)	0	8254	2 1.05
71 EBE/HOY k _a .	DE	650-1000	2.3(14)	0	8455	2
73 KOC/MOI k _a .	EX	913-1473	2.7(14)	0	8354±237	2 1.23
73 SCH1 k _a . Preexponential factor expressed as: A(T/298) ^{-0.907} .	EX	1250-2500	6.95(14)	-0.907	8369	2
74 NAM/TRO k _a . E _a not determined. Within the given T-range k increases from 4.82x10 ⁹ to 9.64x10 ⁹ cm ³ mol ⁻¹ s ⁻¹ .	EX	839-924	4.82(9)			2
75 BOW1 k _a .	ES	1900-2400	6.0(14)	0	8450	2
80 CHI/SKI k _a . H ₂ oxidation in H ₂ /O ₂ /Ar mixtures behind reflected shock-waves. Resonance-absorption Spectroscopy.	EX	925-1825	1.1(14)	0	8107	2
82 PAM/SKI2 k _a . Reaction of O with H ₂ behind reflected shock-waves, in H ₂ /O ₂ /Ar mixtures. Resonance-absorption Spectroscopy. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ . P = (1.16-2.67) atm.	EX	1000-2500	1.2(14)	0	8107	2
71 GAY/PRA ¹⁾ k _b . Expansion channel experiments.	EX	1950-2575	(9.9±5.0)(14)	0	0	3
71 GAY/PRA ¹⁾ k _b . Radical overshoot experiments.	EX	1220-2370	(1.2±0.3)(15)	0	0	3
¹⁾ M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 2.0(N ₂), 18.0(H ₂ O).						
71 HIK/EYR k _b . M = Ar.	EX	298	(5.9±0.7)(15)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 OSB k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.27(Ne), 1.27(He), 1.85(Kr), 2.20(H ₂).	EX	298	2.12(15)			3	
72 AHU/MIC k_b . M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 0.2(Ne), 1.2(He), 1.8(Kr), 2.0(H ₂).	EX	298	(2.18±0.15)(15)			3	
72 JAC/HOU k_b . M = Ar.	EX	948-1125	2.3(15)	0	0	3	
72 KUR2 k_b . M = He.	EX	203-404	2.41(15)	0	-238±46	3	1.18
72 KUR2 k_b . M = He. M-efficiencies relative to He are: 1.0(He), 4.56(N ₂).	EX	226	6.93(15)			3	
72 KUR2 k_b . M = He. M-efficiencies relative to He are: 1.0(He), 1.0(Ar), 3.4(N ₂), 15.7(CH ₄).	EX	298	5.70(15)			3	
72 MOO/ALL k_b . M = He. M-efficiencies relative to He are: 1.00(He), 1.04(Ar), 4.26(H ₂).	EX	297	(5.4±0.2)(15)			3	
72 WES/DEH1 k_b .	EX	298	(6.8±1.0)(15)			2	
73 KOC/MOI k_b . M = H ₂ .	EX	913-1473	3.24(15)	0	-770±101	3	1.02
73 PEE/MAH1 k_b . M = O ₂ .	EX	1900	2.5(15)			3	
74 HAC/HOY2 k_b . M = He.	EX	300	(5.0±1.0)(15)			3	
74 WON/DAV k_b . M = Ar.	EX	220-360	(2.45±0.40)(15)	0	-345±64	3	
74 WON/DAV k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 2.69(N ₂).	EX	220	(1.12±0.07)(16)			3	
74 WON/DAV k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.93(He), 3.0(H ₂), 2.8(N ₂), 22.0(CH ₄).	EX	298	7.73(15)			3	
75 VAS/MAK k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.00(He), 4.08(CO ₂).	RN	300	4.35(15)			3	
76 HAC/WAG k_b . M = He.	EX	293	(9.0±1.0)(15)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 SLA k _b . M = N ₂ . M-efficiencies relative to N ₂ are: 1.0(Ar), Ar(0.67).	ES	964-1075	(3.3±0.6)(15)	0	0	3
77 SLA ²⁾ k _b . M = Ar. Best-fit of all available data.	SE	200-2200	7.05(15)	-1.0	0	3
77 SLA ²⁾ k _b . M _{eff} (N ₂) = 3.1 at 300 K, decreasing to 1.5 1.5 above 1000 K. Best fit all available data. 2) Preexponential factor expressed as: A(T/298) ⁿ .	SE	200-2000	2.05(16)	-1.42	0	3
78 CAM/ROG k _b . M = N ₂ . Discharge-flow. P(Total) = (0.2-0.5) kPa.	EX	425	(1.2±0.2)(13)			3
78 HAC/WAG k _b . M = He. Isothermal discharge-flow reactor. P = 3.8 torr.	EX	293	(9.0±1.0)(15)			3
79 ISH/SUG2 k _b . M = H ₂ . Pulse-radiolysis. Absorption-spectroscopy. P = 747 torr. H ₂ + 0.93 torr. O ₂ .	EX	298	(1.09±0.22)(16)			3
79 MOR/HEI k _b /k _{ref} . HCHO photolysis at 313 nm. M = O ₂ + N ₂ + 2CO + 3HCHO. k _{ref} : HCHO + H → CHO + H ₂	RL	298	(6.1±1.8)(5)			3/2
80 CHI/SKI k _b . M = Ar. H ₂ oxidation in H ₂ /O ₂ /Ar mixtures behind reflected shock-waves. Resonance-absorption Spectroscopy.	EX	1000	7.0(14)			3
82 PAM/SKI2 k _b . M = Ar. Reaction of O with H ₂ behind reflected shock-waves in H ₂ /O ₂ /Ar mixtures. Resonance-absorption spectroscopy. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ . P = (1.16-2.67) atm.	EX	1000-2500	4.5(14)	0	505	3
H + O₂(¹Δ_g) → OH + O (principal channel)						
Hydrogen atom + Oxygen molecule						
73 SCH/SCH2	EX	300	(1.51±0.30)(10)			2
82 CUP/TAK Discharge-flow apparatus. EPR-spectrometry. O ₂ (¹ Δ _g) generated by microwave-discharge of O ₂ /Ar mixtures. H atoms generated by microwave-discharge of H ₂ /Ar mixtures.	EX	300-431	(8.79±2.95)(12)	0	2013±101	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
D + O₂ (+ M) → OD + O (+ M) (a)							
→ DO₂ (+ M) (b)							
Deuterium atom + Oxygen molecule							
75 APP/APP k _a . Data fit.	ES	1700-3100	3.13(14)	0	9935	2	1.3
80 CHI/SKI k _a . D ₂ oxidation in D ₂ /O ₂ /Ar mixtures behind reflected shock-waves. Resonance-absorption.	EX	1700-2200	1.6(13)	0	7554	2	
82 PAM/SKI2 k _a . Reaction of O with D ₂ behind reflected shock-waves in D ₂ /O ₂ /Ar mixtures. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ . Resonance-absorption. P = (1.16-2.67) atm.	EX	1000-2500	5.8(13)	0	7554	2	
75 VAS/MAK k _b . M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 1.0(He), 4.0(CO ₂).	EX	300	4.35(15)			3	
79 ISH/SUG2 k _b . M = D ₂ . Pulse-radiolysis. Absorption-Spectroscopy. P = 748 torr. (D ₂ + O ₂)	EX	298	(1.05±0.47)(16)			3	
80 CHI/SKI k _b . M = Ar. D ₂ oxidation in D ₂ /O ₂ /Ar mixtures behind reflected shock-waves. Resonance-absorption.	EX	1000	1.6(14)			3	
82 PAM/SKI2 k _b . M = Ar. Reaction of O with D ₂ behind reflected shock-waves in D ₂ /O ₂ /Ar. Resonance-absorption. [O] = 5.42x10 ⁸ -3.49x10 ¹² molec.cm ⁻³ . P = (1.16-2.67) atm.	EX	1000-2500	2.2(14)	0	505	3	
H + O₃ → OH + O₂ (a)							
→ HO₂ + O (b)							
Hydrogen atom + Ozone							
77 CLY/MON k _a .	EX	298-638	5.95(13)	0	224±26	2	1.26
77 SHA k _a . Preexponential factor expressed as: A(T/298) ^{0.75} .	ES	250-2000	1.64(13)	0.75	0	2	
78 LEE/MIC2 k _a . Flash-photolysis. Resonance-fluorescence.	EX	219-360	(8.01±1.93)(13)	0	449±58	2	
79 KEY k _a . Discharge-flow. Resonance-fluorescence. OH is vibrationally excited, with v ≤ 9.	EX	196-424	(9.03±1.08)(11)	0	499±32	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 FOR/WIE k _a + k _b . M = He. Laser photolysis of O ₃ /H ₂ mixtures. H atoms produced by the reaction: O(¹ D) + H ₂ → OH + H. P(H ₂) = 110 mtorr. P(He) = 20 torr. P(O ₃) = (1.7-3.8) mtorr.	EX	298	(1.69±0.06)(13)			2	
H + H (+ M) → H₂ (+ M)							
Hydrogen atom							
71 BEN/BLA M = H ₂ . M-efficiencies relative to H ₂ are: 1.0(H ₂), 1.1(N ₂), 1.3(He), 1.7(Ar), 1.6(CO ₂), 1.7(CH ₄), 9.0(N ₂ O).	EX	298	(3.4±0.5)(15)			3	
71 GAY/PRA ¹⁾ Expansion channel experiments.	EX	1950-2575	3.3(14)	0	0	3	1.97
71 GAY/PRA ¹⁾ Radical overshoot experiments.	EX	1220-2370	(3.8±0.5)(14)	0	0	3	
¹⁾ M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 1.0(N ₂), 6.0(H ₂ O).							
73 AZA/BOR M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.31(He).	EX	298	(4.5±0.7)(15)			3	
73 TEN/WIN ²⁾ M = NH ₃ . Based on k _{ref} reported in 71 BEN/BLA.	RN	298	(4.0±0.09)(16)			3	
73 TEN/WIN ²⁾ M = NH ₃ . Based on k _{ref} estimated by: Ham, D.Trainer, D.W., and Kaufman, F., in J. Chem. Phys. 53, 4395(1079).	RN	298	5.14(16)			3	
²⁾ Determined by adding NH ₃ to He carrier gas, then using the literature values for the H atom recombination in presence of He, to calculate the k in presence of NH ₃ . k _{ref} : H + H + He.							
73 TRA/HAM M = He. M-efficiencies relative to He are: 1.00(He), 1.54(H ₂), 2.28(Ar).	EX	77	(4.35±0.54)(15)			3	
73 TRA/HAM M = He. M-efficiencies relative to He are: 1.00(He), 1.16(H ₂), 1.31(Ar).	EX	298	(2.54±0.15)(15)			3	
74 MAL/OWE M = Ar.	EX	1300-1700	1.0(15)	0	0	3	1.20

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 WAL/KAU ³⁾ M = H ₂ . n = 0 assumed.	EX	77-298	2.21(15)	0	-86	3	1.1
75 WAL/KAU ³⁾ M = H ₂ .	EX	77-298	2.94(15)	-0.6	0	3	1.1
75 WAL/KAU ³⁾ M = CO ₂ . n = 0 assumed.	EX	175-295	1.01(15)	0	-523	3	1.1
75 WAL/KAU ³⁾ M = CO ₂ .	EX	175-295	5.80(15)	-2.27	0	3	1.1
³⁾ A-factors recalculated from the E _a (or the given n of the T ⁻ⁿ factor) and the experimental k at 298 (or 295) K. The preexponential factors expressed as: A(T/298) ⁿ in all the expressions with n ≠ 0.							
75 WAL/KAU M = H ₂ . M-efficiencies relative to H ₂ are: 1.00(H ₂), 0.65(He), 1.48(Ar), 2.97(N ₂), 3.99(CH ₄).	EX	77	(6.71±0.80)(15)			3	
75 WAL/KAU M = H ₂ . M-efficiencies relative to H ₂ are: 1.00(H ₂), 0.87(He), 1.13(N ₂), 1.14(Ar), 1.89(CH ₄), 2.02(CO ₂), 2.41(SF ₆).	EX	298	(2.94±0.15)(15)			3	
76 LYN/SCH M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.61(Ne), 0.72(He), 0.83(Ar), 0.89(H ₂), 1.06(Kr).	EX	298	(3.48±0.51)(15)			3	
77 MIT/LER M = He. About 25% p-H ₂ formed.	EX	297	(2.10±0.07)(15)			3	
78 HAR/KUM ⁴⁾ M = H ₂ . In the presence of H ₂ O vapor traces.	EX	298	(5.44±1.09)(15)			3	
78 HAR/KUM ⁴⁾ M = H ₂ . In the absence of H ₂ O vapor traces.	EX	298	(7.62±2.54)(14)			3	
⁴⁾ Microwave discharge-flow system.							
D + D (+ M) → D₂ (+ M)							
Deuterium atom							
73 AZA/BOR M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.38(He).	EX	298	(2.90±0.54)(15)			3	
73 TRA/HAM ¹⁾	EX	77	5.5(15)			3	1.1
73 TRA/HAM ¹⁾	EX	298	2.2(15)			3	1.1
¹⁾ M = D ₂ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + H₂(v=1) → H₂ + H						
Hydrogen atom + Hydrogen molecule						
78 GOR/IVA1 ¹⁾	EX	300	(3.11±0.12)(12)			2
78 GOR/IVA1 ¹⁾	EX	356	(5.61±0.48)(12)			2
¹⁾ Hydrogen maser storage-bulb. Mass-spectrometry. [H ₂] = (0.5-6.5)×10 ¹³ molec.cm ⁻³ .						
H + HD → H₂ + D						
Hydrogen atom + Deuterium hydride						
72 NIK/MAI	CO	1000	(1.39±0.12)(13)			2
H + HD(v=1) → HD + H (a) → H₂ + D (b)						
Hydrogen atom + Deuterium hydride						
78 GOR/IVA1 ¹⁾	EX	300	(4.40±2.05)(12)			2
78 GOR/IVA1 ¹⁾	EX	356	(3.13±1.08)(12)			2
¹⁾ k _a + k _b . Hydrogen maser storage-bulb. Mass-spectrometry. [H ₂] = (0.5-6.5)×10 ¹³ molec.cm ⁻³ .						
H + D₂ → HD + D						
Hydrogen atom + Deuterium molecule						
72 NIK/MAI	CO	1000	(2.77±0.30)(13)			2
75 APP/APP	EX	1860	4.01(12)			2
75 APP/APP	EX	2680	9.40(12)			2
75 APP/APP	EX	2730	1.00(13)			2
76 PRA/ROG1	EX	274-1220	2.01(11)	3.21	2851±88	2 3.39
The preexponential factor expressed as: A(T/298) ^{3.21} .						
H + D₂(v=1) → HD + D						
Hydrogen atom + Deuterium molecule						
75 GOR/IVA ¹⁾	EX	470	(1.42±0.18)(10)			2
[H ₂] = [D ₂] = (0.1-1.0) ¹⁴ molec.cm ⁻³ .						
78 GOR/IVA1 ¹⁾	EX	300	(5.06±0.60)(11)			2
78 GOR/IVA1 ¹⁾	EX	356	(5.48±0.90)(11)			2
[H ₂] = [D ₂] = (0.5-6.5)×10 ¹³ molec.cm ⁻³ .						
¹⁾ Hydrogen maser storage-bulb.. Mass-spectrometry.						
D + H₂ → HD + H						
Deuterium atom + Hydrogen molecule						
72 NIK/MAI	CO	1000	(3.67±0.36)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 MIT/LER The preexponential factor expressed as: $A(T/298)^2$.	EX	167-346	(1.46±0.09)(12)	2.0	2698±20	2	
75 APP/APP	EX	2600	1.54(13)			2	
76 PRA/ROG1 The preexponential factor expressed as: $A(T/2.5198)^{2.51}$.	EX	274-1220	7.77(11)	2.51	2491±70	2	2.75
D + H₂(v=n) → DH + H							
Deuterium atom + Hydrogen molecule							
82 GLA/CHA ¹) v = 0.	EX	297	(1.51±0.60)(8)			2	
82 GLA/CHA ¹) v = 1.	EX	297	(5.90±1.81)(11)			2	
¹) Discharge-flow system. EPR-spectrometry.							
D + HD → D₂ + H							
Deuterium atom + Deuterium hydride							
72 NIK/MAI	CO	1000	(1.87±0.18)(13)			2	
H + OH (+ M) → H₂O (+ M)							
Hydrogen atom + Hydroxyl							
72 FRI/SUT M = O ₂ , N ₂ . Rate constant expressed as: $k[M] = 4.4 \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$.	ES	2130	4.4(10)			2	
77 ZEL/ERL	EX	230-300	1.56(10)	0	0	2	1.2
71 GAY/PRA Expansion channel experiments.	EX	1950-2575	(2.4±0.8)(15)	0	0	3	
71 GAY/PRA Radical overshoot experiments.	EX	1220-2370	(2.7±0.7)(15)	0	0	3	
¹) M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 4.0(N ₂), 18.0(H ₂ O).							
77 ZEL/ERL M = He. The preexponential factor expressed as: $A(T/298)^{-2.6}$.	EX	230-300	(5.76±4.02)(16)	-2.6	0	3	
77 ZEL/ERL M = He. M-efficiencies relative to He are: 1.0(He), 1.5(Ar), 3.2(N ₂), 6.0(CO ₂).	EX	300	(5.44±1.45)(16)			3	
D + OH → OD + H							
Deuterium atom + Hydroxyl							
75 MAR/KAU2 Discharge-flow. UV Resonance-fluorescence.	EX	295	(7.83±1.81)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 HOW/SMI Laser flash-photolysis. Time-resolved Resonance-fluorescence. OH generated by pulse Laser-photolysis of HONO ₂ or H ₂ O. D atom generated by D ₂ microwave discharge. The preexponential factor expressed as: A(T/298) ^{-0.63} .	EX	300-515	(3.15±0.50)(13)	-0.63	0	2
H + OH + OH → H₂O + OH(²Σ)						
Hydrogen atom + Hydroxyl						
74 DAV/MCG	EX	1740-1860	(8.34±0.33)(15)	0	0	3
H + OH + CO → HCHO + O						
Hydrogen atom + Hydroxyl + Carbon monoxide						
78 SME/PAV Shock-waves. Non-Arrhenius expression. 1) k = 4.35x10 ²⁰ (1/T) cm ⁶ mol ⁻² s ⁻¹ .	EX	1500-3500	¹⁾			3
H + HO₂ → H₂ + O₂ (a) → OH + OH (b) → H ₂ O + O (c)						
Hydrogen atom + Hydroperoxo						
71 BEN/BLA k _a /k _b . Estimated ratio.	RL	298	(7.5±2.5)(-1)			2/2
72 WES/DEH1 k _a /(k _a + k _b + k _c). Estimated ratio.	RL	298	6.2(-1)			2/2
74 BAL/FUL1 k _a /k _b . Reaction vessel in electric furnace. Second limit measurement.	RL	773	1.7(-1)			2/2
74 BAL/FUL1 k _a + k _b . Reaction vessel in electric furnace. Second limit measurement.	ES	300-773	3.1(14)	0	868	2
76 HAC/WAG k _a /(k _a + k _b + k _c).	RL	293	2.9(-1)			2/2
76 HAC/WAG k _a .	RN	293	(6.7±1.5)(12)			2
77 SHA k _a . The preexponential factor expressed as: A(T/298) ^{0.75} .	ES	250-2000	8.25(12)	0.75	0	2
78 HAC/WAG ¹⁾ k _a /k _b .	RL	293	4.2(-1)			2/2
78 HAC/WAG ¹⁾ k _a /(k _a + k _b + k _c).	RL	293	2.9(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 HAC/WAG ¹⁾ k _a .	RN	293	(1.0±0.5)(13)				2
1) Isothermal discharge-flow reactor. P = 3.8 torr.							
82 SRI/QIU k _a . Discharge-flow reactor. Laser-induced Fluorescence. UV-Resonance-Fluorescence. HO ₂ generated by reacting F with H ₂ O ₂ . F atoms generated by dissociation of CF ₄ in a microwave-discharge. H and O atoms generated by dissociation of H ₂ and O ₂ in a microwave-discharge. [NO] ~ 2x10 ¹⁴ molec.cm ⁻³ . P(He) ~ 2.5 torr. [H] ₀ = [O] ₀ ~ (4-5)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)x10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8x10 ¹² molec.cm ⁻³ .	EX	296	(4.03±2.04)(12)				2
72 DAY/DIX ²⁾	RL	300-1800	(6.5±1.0)	0	0		2/2
73 DAY/THO ²⁾	RL	300-1050	(6.5±1.0)	0	0		2/2
2) (k _b + k _c)/k _a . Estimated ratio.							
72 WES/DEH1 k _b /(k _a + k _b + k _c). Estimated ratio.	RL	298	2.7(-1)				2/2
76 HAC/WAG k _b /(k _a + k _b + k _c).	RL	293	6.9(-1)				2/2
76 HAC/WAG k _b .	RN	293	(1.6±0.8)(13)				2
77 COL/NAE ³⁾ k _{ref} : H + CH ₃ CHO → H ₂ + CH ₃ CO	RL	1113	2.5(-2)				2/2
77 COL/NAE ³⁾ k _{ref} : HO ₂ + CH ₃ CHO → H ₂ O ₂ + CH ₃ CO	RL	1113	2.9(-2)				2/2
77 COL/NAE ³⁾ k _{ref} : H ₂ O ₂ + M → OH + OH + M	RL	1113	3.1(-2)				2/2
3) k _b /k _{ref} .							
77 SHA k _b . The preexponential factor expressed as: A(T/298) ^{0.75} .	ES	250-2000	8.25(12)	0.75	0		2
78 HAC/WAG ⁴⁾ k _b /(k _a + k _b + k _c).	RL	293	6.9(-1)				2/2
78 HAC/WAG ⁴⁾ k _b .	RN	293	(2.5±1.0)(13)				2
4) Isothermal discharge-flow reactor. P = 3.8 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 SRI/QIU k _b . Discharge-flow reactor. Laser-induced Fluorescence. UV-Resonance-Fluorescence. HO ₂ generated by reacting F with H ₂ O ₂ . F, H and O atoms generated by dissociation of CF ₄ , H ₂ and O ₂ , respectively, in a microwave-discharge. P(He) ~ 2.5 torr. [NO] ~ 2x10 ¹⁴ molec.cm ⁻³ . [H] ₀ = [O] ₀ ~ (4-5)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)x10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8x10 ¹² molec.cm ⁻³ .	EX	296	(3.85±0.60)(13)			2
72 WES/DEH1 k _c /(k _a + k _b + k _c). Estimated ratio.	RL	298	1.1(-1)			2/2
76 HAC/WAG k _c /(k _a + k _b + k _c).	RL	293	2.0(-2)			2/2
76 HAC/WAG k _c .	RN	293	5.0(11)			2
78 HAC/WAG ⁵⁾ k _c /(k _a + k _b + k _c).	RL	293	2.0(-2)			2/2
78 HAC/WAG ⁵⁾ k _c . Upper-limit k.	RN	293	≤7.0(11)			2
⁵⁾ Isothermal discharge-flow. P = 3.8 torr.						
82 SRI/QIU k _c . Discharge-flow. Laser-induced Fluorescence. UV-Resonance-Fluorescence. HO ₂ generated by reacting F with H ₂ O ₂ . F, H and O atoms generated by dissociation of CF ₄ , H ₂ and O ₂ , respectively, in a microwave discharge. P(He) ~ 2.5 torr. [NO] ~ 2x10 ¹⁴ molec.cm ⁻³ . [H] ₀ = [O] ₀ ~ (4-5)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)x10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8x10 ¹² molec.cm ⁻³ .	EX	296	(1.81±0.90)(12)			2
77 HAC/PRE k _a + k _b + k _c . Isothermal flow.	EX	293	(3.6±1.0)(13)			2
78 PRE k _a + k _b + k _c . Laser Magnetic Resonance Spectroscopy.	EX	293	(3.2±1.0)(13)			2
79 HAC/PRE1 k _a + k _b + k _c . Isothermal flow. Laser Magnetic Resonance Spectrometry. P(Total) = (130-800) Pa.	EX	293	(2.8±0.6)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 THR/WIL2 $k_a + k_b + k_c$. Laser magnetic Resonance Spectrometry.	EX	298	(3.01±0.78)(13)			2
82 SRI/QIU $k_a + k_b + k_c$. Discharge-flow. Laser-induced Fluorescence. UV-Resonance-Fluorescence. HO ₂ radicals generated by reacting F with H ₂ O ₂ . F, H and O atoms generated by dissociation of CF ₄ , H ₂ , and O ₂ , respectively, in a microwave-discharge. [H] ₀ = [O] ₀ ~ (4-5)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] = (1-10)x10 ¹³ molec.cm ⁻³ . [H ₂ O ₂] = 8x10 ¹² molec.cm ⁻³ . [NO] ~ 2x10 ¹⁴ molec.cm ⁻³ . P(He) ~ 2.5 torr.	EX	296	(4.46±0.72)(13)			2
H + H₂O → H₂ + OH Hydrogen atom + Water						
79 COH/WES Critical review. $k_1 = Kk_{-1}$. The preexponential factor expressed as: $A(T/298)^{1.2}$. $\Delta \log k = 0.1$ at 300 K, and 0.4 at 2000 K.	RE	250-3000	9.52(12)	1.2	9610	2
H + H₂O₂ → H₂ + HO₂ (a) → OH + H₂O (b) Hydrogen atom + Hydrogen peroxide						
72 VOL/GOR k_b/k_a .	RL	298	(3.0±1.0)			2/2
73 GOR k_a .	ES	298	(2.41±1.20)(8)			2
74 GOR/VOL k_a .	ES	298	(1.87±0.48)(9)			2
75 KLE/PAY $k_a + k_b$. Channel (b) assumed to be predominant.	EX	283-353	(3.13±1.20)(12)	0	1399±141	2
72 GOR/VOL k_b/k_a . (Corrected rate ratio.)	RL	298	(2.0±1.0)			2/2
73 GOR k_b/k_a .	RL	298	(3.0±1.0)			2/2
73 GOR k_b .	ES	298	(7.23±0.36)(8)			2
74 GOR/VOL k_b/k_a .	RL	298	(1.86±0.14)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 GOR/VOL k_b .	ES	298	(3.4±0.84)(9)			2
75 MEA/HEI k_b/k_a .	RL	298	1.3			2/2
D + H₂O₂ → HD + HO₂ (a)						
→ OH + HDO (b)						
Deuterium atom + Hydrogen peroxide						
71 ALB/HOY $k_a + k_b$.	EX	294-464	7.0(12)	0	2114±201	2
H + SO₂ → HSO₂						
Hydrogen atom + Sulfur dioxide						
78 GOR/IVA2 ¹⁾	EX	305	1.81(11)			2
78 GOR/IVA2 ¹⁾	EX	375	2.23(11)			2
¹⁾ Based on collision-induced shifts and HF-transition line broadening in H atoms.						
H + SH → H₂ + S						
Hydrogen atom + Mercapto						
72 LAN/OLD Upper-limit k.	ES	293	≤6.02(12)			2
73 BRA/TRU	EX	298	2.5(13)			2
75 CUP/GLA	EX	295	(1.51±0.48)(13)			2
79 NIC/AMO Radio-frequency pulse. Kinetic spectroscopy. Computer simulation. High-vacuum. P = (0.1-2) torr.	DE	295	(1.3±0.2)(13)			2
H + H₂S → H₂ + SH						
Hydrogen atom + Hydrogen sulfide						
71 KUR/PET1	EX	190-464	(7.77±0.90)(12)	0	860±30	2
72 ROM/SCH	EX	298	(2.29±0.24)(11)			2
73 BRA/TRU	EX	298	5.0(11)			2
77 FRA/ROG Conventional static system.	EX	808-937	2.75(13)	0	330±220	2 1.78
79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum system. Computer simulation. P = (0.1-2) torr.	DE	295	(5.0±0.4)(11)			2
80 HUS/SLA1 Time-resolved Resonance-Fluorescence.	EX	300	(5.18±0.30)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 ROT/LOE1 Thermolysis of H ₂ S behind reflected shock-waves. Atomic-resonance Absorption-Spectroscopy. P(Total) = (1350-15000) torr. [H ₂ S] = (0.6-4.9)x10 ¹⁵ molec.cm ⁻³ . [Ar] = (5.0-8.0)x10 ¹⁸ molec.cm ⁻³ .	EX	1965-2560	1.08(13)	0	1500	2	
D + D ₂ S → D ₂ + SD Deuterium atom + Hydrogen sulfide (D ₂ S)							
80 HUS/SLA1 Time-resolved Resonance-Fluorescence.	EX	300	(4.76±0.24)(11)			2	
H + N (+ M) → NH (+ M) Hydrogen atom + Nitrogen atom							
73 BRO Central k value by averaging: k < (6.4±1.5)x10 ⁻³² cm ⁶ molec ⁻² s ⁻¹ and k > (3.1±1.0)x10 ⁻³² cm ⁶ molec ⁻² s ⁻¹ .	EX	298	(1.82±1.05)(16)			3	
H + N ₂ → NH + N Hydrogen atom + Nitrogen molecule							
78 ROO/HAN Shock-waves. The preexponential factor expressed as: A(T/298) ^{0.5} .	ES	1700-3000	5.18(13)	0.5	71465	2	
H + NO (+ M) → OH + N (+ M) Hydrogen atom + Nitrogen oxide (NO)							
75 BRA/CRA ¹⁾	DE	2530-3020	3.5(14)	0	23937	2	
75 DUX/PRA ¹⁾	DE	2200-3250	2.6(14)	0	24560	2	
¹⁾ Optimization based on a proposed mechanism.							
75 FLO/HAN Best fit to the experimental data.	EX	2403-4500	1.34(14)	0	24761±403	2	1.15
75 KOS/AND Data-fit to a proposed mechanism.	ES	2000-4000	3.16(13)	0	24157±151	2	2.0
76 AND/ASA Reevaluation of the experimental data reported in 75 KOS/AND by using computer simulation.	DE	2300-3500	5.01(13)	0	24509	2	1.41
77 FLO/HAN Best data-fit to a proposed mechanism.	EX	2415-4200	2.22(14)	0	25415±302	2	1.20

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 MCC/KRU ²⁾	EX	1750-2040	1.74(14)	0	24761	2 1.58
77 MCC/KRU ²⁾	RE	1750-2040	1.71(14)	0	24560	2
Based on a curve fit of all previous rate constants. Recommended k.						
²⁾ Flow reactor.						
Same data given in 76 MCC/KRU.						
77 OKA/SIN2	EX	298-477	(4.61±0.16)(15)	0	-363±13	2
M = H ₂ .						
Photomultiplier with lock-in amplifier.						
81 FOR ³⁾	EX	313	5.01(14)			2
M = N ₂ . P >400 atm.						
81 FOR ³⁾	EX	313	1.50(14)			2
M = Ar. P <100 atm. Extrapolation by using the Cassel curve method of Troe.						
³⁾ Steady-state quasi-monochromatic Photolysis of NO/HI mixtures. Limiting high-pressure k's.						
71 HIK/EYR	EX	298	(1.4±0.2)(16)			3
M = H ₂ .						
71 OSB	EX	298	1.40(16)			3
M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 0.56(Ne), 1.11(He), 1.40(Kr), 1.63(H ₂).						
72 AHU/MIC	EX	298	(1.41±0.04)(16)			3
M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 0.5(Ne), 1.1(He), 1.4(Kr), 1.6(H ₂).						
73 ATK/CVE ⁴⁾	EX	285-390	8.9(15)	0	-272±75	3
73 ATK/CVE ⁴⁾	EX	298	(2.150±0.13)(16)			3
⁴⁾ M = H ₂ .						
75 CAM/HAN2	EX	392	(8.7±0.7)(15)			3
M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.64(N ₂).						
77 OKA/SIN1	EX	298	(1.56±0.06)(16)			3
M = H ₂ .						
77 OKA/SIN2 ⁵⁾	EX	298	(1.55±0.23)(16)			3
M = H ₂ .						
77 OKA/SIN2 ⁵⁾	EX	298	(1.91±0.38)(16)			3
M = NO.						
⁵⁾ Photomultiplier with lock-in amplifier.						
79 ISH/SUG2	EX	298	(1.66±0.22)(16)			3
M = H ₂ . Pulse-radiolysis.						
Absorption-spectroscopy.						
P = (100-300) torr. H ₂ + (0.05-0.65) torr. NO						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
D + NO (+ M) → DNO (+ M)							
Deuterium atom + Nitrogen oxide (NO)							
79 ISH/SUG2 M = D ₂ . Pulse-radiolysis. Absorption-spectroscopy. P = (100-900) torr. (D ₂ + NO)	EX	298	(1.60±0.36)(16)			3	
H + NO₂ → OH + NO							
Hydrogen atom + Nitrogen oxide (NO ₂)							
76 WAG/WEL	EX	240-460	(4.3±1.8)(14)	0	505±84	2	
77 BEM/CLY	EX	298	(6.81±1.39)(13)			2	
77 CLY/MON	EX	298-653	2.89(14)	0	174±31	2	1.21
79 MIC/NAV2 T-independent. Mean value of two techniques: Flash-photolysis-, and Discharge-flow- Resonance-fluorescence.	EX	195-400	(8.49±1.57)(13)	0	0	2	
81 AGR/MAN Flowing-afterglow apparatus. Rotationless Ein- stein coefficient of Rosmus. P(Ar) = 0.7 torr.	EX	300	7.53(13)			2	
H + N₂O → OH + N₂ (a) → NH + NO (b)							
Hydrogen atom + Nitrogen oxide (N ₂ O)							
73 BAL/GET k _a /k _{ref} . k _{ref} : H + O ₂ → OH + O.	RL	773	(6.4±0.7)(-1)			2/2	
73 BAL/GET ¹⁾	RN	773	2.6(9)			2	1.4
73 BAL/GET ¹⁾ ¹⁾ k _a .	SE	460-2500	7.6(13)	0	7599±503	2	
73 WAL1 k _a /k _{ref} . k _{ref} : H + O ₂ → OH + O.	RL	773	(6.4±0.07)(-1)			2/2	
73 WAL1 ²⁾	RN	773	2.6(10)			2	1.4
73 WAL1 ²⁾ Present and independent data combined.	SE	700-2503	7.6(13)	0	7599±503	2	
²⁾ k _a .							
75 ALB/HOY k _a .	EX	718-1111	(2.2±0.7)(14)	0	8709±349	2	
77 BAL/VAN k _a . Supersonic molecular beam. Mass-spectrometry. P = 40 torr.	EX	1000-1700	(6.0±2.0)(13)	0	6593	2	
78 DEA/STE k _a . M = Ar. Reflected shock waves. Best fit.	EX	1950-2850	1.81(15)	0	13592	2	
79 GLA/QUY k _a . Discharge-flow shock-tube.	EX	1473-2710	(3.82±0.66)(13)	0	8505±377	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 QUY k _a . Shock-tube technique. P < 760 torr.	EX	1475-2875	(3.26±0.47)(13)	0	8153±302	2	
80 DEA/JOH1 k _a . HCHO Decomposition behind shock-waves. Best data fit. Total conc. = 5x10 ¹⁸ molec.cm ⁻³ .	EX	1700-2500	3.31(14)	0	5281	2	
80 MUR/BOR1 ³⁾	RN	1550	9.77(11)			2	
80 MUR/BOR1 ³⁾	RN	1923	1.26(12)			2	
³⁾ k _a . Oxidative pyrolysis of CH ₄ behind reflected shock-waves, initiated by the N ₂ O decomposition. Other k values are given for various T's within (1550-1923) K range. E _a not given. Determined relative to the reaction:							
$H + CH_4 \rightarrow H_2 + CH_3$							
78 BOR/ZAM k _b . Static system. Reflected shock-waves.	EX	850-2000	6.31(13)	0	14595±755	2	2.0
H + N₂O(v=3) → OH + N₂ Hydrogen atom + Nitrogen oxide (N ₂ O)							
77 GER/EGO Upper-limit k.	EX	298	<6.02(10)			2	
H + NH → H₂ + N Hydrogen atom + Imidogen							
81 MOR2 Premixed H ₂ /O ₂ /Ar flames. Laser-fluorescence. P = 760 torr.	EX	1790	~3.01(13)			2	2.0
H + NH₂ (+ M) → H₂ + NH (+ M) (a) → NH₃ (+ M) (b) Hydrogen atom + Amidogen							
71 BOY/WIL k _a . Radiolysis of gaseous NH ₃ . P(NH ₃) = 700 torr.	ES	298	(2.9±0.7)(12)			2	
79 DOV/NIP k _a . Pyrolysis behind reflected shock-waves.	RN	2500-3000	6.17(13)	0	2630	2	
81 YUM/ASA k _a . M = Ar. Thermolysis of NH ₃ behind incident shock-waves. Vacuum-UV Absorption-Spectroscopy. [NH ₃] ₀ = (1.2-2.4)x10 ¹⁴ molec.cm ⁻³ . [Ar] = (0.2-1.8)x10 ¹⁸ molec.cm ⁻³ .	EX	2450-3020	3.02(13)	0	4308	2	
71 BOY/WIL k _b . Radiolysis of gaseous NH ₃ . P(NH ₃) = 700 torr.	ES	298	(1.8±0.4)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 PAG/ERI k _p . Gaseous NH ₃ pulse-radiolysis.	EX	349	1.6(13)			2	
71 GOR/MUL k _p . Unreported T assumed to be 298 K.	EX	298	2.2(18)			3	
H + NH₃ → H₂ + NH₂							
Hydrogen atom + Ammonia							
74 DOV/NIP	EX	1500-2150	2.75(13)	0	8757±654	2	1.45
81 YUM/ASA M = Ar. Thermolysis of NH ₃ behind incident shock-waves. Vacuum-UV Absorption-Spectroscopy. [NH ₃] ₀ = (0.6-1.8)×10 ¹⁵ molec.cm ⁻³ . [Ar] = (0.1-1.2)×10 ¹⁹ molec.cm ⁻³ .	EX	1860-2480	1.24(14)	0	10820±5184	2	11.0
H + NH₂NH → NH₂ + NH₂							
Hydrogen atom + Hydrazyl							
71 GEH/HOY	EX	300	(1.6±0.8)(12)			2	
H + NH₂NH₂ → H₂ + NH₂NH							
Hydrogen atom + Hydrazine							
71 FRA/JON	EX	300-540	(1.5±0.3)(12)	0	654±101	2	
71 GEH/HOY	EX	213-473	1.3(13)	0	1258	2	
76 STI/PAY	EX	228-400	(5.94±0.70)(12)	0	1198±50	2	
H + HN₃ → NH₂ + N₂							
Hydrogen atom + Hydrazoic acid							
73 LEB/COM	EX	300-460	1.53(13)	0	2315	2	
H + HNO → H₂ + NO							
Hydrogen atom + Nitrosyl hydride							
72 SMI	EX	2100	(2.35±1.14)(12)			2	
75 CAM/HAN2 k _{ref} : O + HNO → OH + NO. Upper-limit ratio.	RL	425	≤8.86(-3)			2/2	
78 WAS/AKI Fast flow. Lower-limit k. Photoionization Mass-spectrometer.	EX	298	>9.64(11)			2	
80 DOD/ZEL High-frequency discharge. Mass-spectrometry.	EX	295	(7.23±3.00)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
H + HONO₂ → products							
Hydrogen atom + Nitric acid							
74 CHA/WAY Upper-limit k.	EX	300	≤1.20(9)				2
H + HO₂NO₂ → products							
Hydrogen atom + Peroxynitric acid							
81 TRE/BAR ¹⁾	EX	248-315	(1.48±0.21)(10)	0	0		2
81 TRE/BAR ¹⁾	EX	238	(3.86±0.84)(10)				2
¹⁾ Stirred-flow reactor. Modulated molecular-beam Spectrometer. P(Total) = (1-3) torr.							
H + CO (+ M) → CHO (+ M)							
Hydrogen atom + Carbon monoxide							
78 GOR/IVA2 ¹⁾	EX	305	>1.51(10)				2
78 GOR/IVA2 ¹⁾	EX	375	>2.41(11)				2
¹⁾ Collision-induced shifts. HF-transition line broadening in H atoms. Lower-limit k's.							
71 BEN/BLA M = H ₂ . Upper-limit k.	EX	298	≤1.2(14)				3
71 HIK/EYR M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.54(H ₂).	EX	298	(2.6±0.4)(13)				3
72 AHU/MIC M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 1.0(He), 0.8(Ne), 1.1(Kr), 1.3(H ₂).	EX	298	(2.18±0.25)(15)				3
72 BAL/JAC M = H ₂ .	DE	773	2.3(14)				3
73 AZA/AND M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 2.0(CO).	EX	298	(3.99±2.18)(13)				3
80 HOC/SWO1 M = H ₂ . M-efficiencies relative to H ₂ are: 1.00(H ₂), 0.95(CO), 1.53(CH ₄). H ₂ Flash-photolysis in presence of CO. P = 760 torr.	EX	298	(3.8±0.4)(13)				3
H + CO + OH → HCHO + O							
Hydrogen atom + Carbon monoxide + Hydroxyl							
78 SME/PAV Shock-waves. Non-Arrhenius expression: ¹⁾ k = 4.35x10 ²⁰ (1/T) cm ⁶ mol ⁻² s ⁻¹	EX	1500-3500	¹⁾				3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
H + CO₂ → OH + CO						
Hydrogen atom + Carbon dioxide						
75 VAN/PEE k ₁ = k ₋₁ K.	DE	650-1800	4.8(14)	0	12582	2
78 WAW/ZIE H ₂ dissociation in a quartz vessel using the system ¹⁴ CO ₂ /CO/H ₂ . P(Total) = (100-200) torr.	EX	1013-1243	9.0(13)	0	12028	2
H + CH → H₂ + C						
Hydrogen atom + Methylidyne						
82 GRE/HOM2 Reaction of the Ethyne/O/H system, diluted in N ₂ /He, in a discharge-flow reactor. Resonance-fluorescence. O atoms generated by reacting N with NO. P = 2 torr.	EX	298	≈3.0(13)			2
H + CH₂ → H₂ + CH						
Hydrogen atom + Methylene						
82 GRE/HOM1 Reaction of the CH=CH/O/H system diluted in N ₂ /He, in a discharge-flow reactor. Resonance-fluorescence. O atoms generated by reacting N with NO. H atoms produced by a discharge of the mixture H ₂ /He. Best data fit. P = 2 torr.	EX	298	(5.0±1.0)(13)			2
H + CH₃ (+ M) → CH₄ (+ M)						
Hydrogen atom + Methyl						
72 TEN/JON Data-fit to a proposed mechanism.	CO	303-603	1.17(12)	0	25	2
74 CAM/MAR Average of three k's at 8, 12, and 16 torr., over the given T-range.	EX	503-753	(1.64±0.55)(12)	0	0	2
77 CHE/LEE	EX	308	1.5(14)			2
77 CHE/YEH Extrapolated limiting high-pressure k.	ES	308	(2.0±0.9)(14)			2
79 SEP/MAR ¹⁾ P(Ar) ~ 14 torr.	EX	750	2.82(12)			2
79 SEP/MAR ¹⁾ P(Ar) = 7.4 torr.	EX	768-818	1.58(12)			2
¹⁾ Discharge-flow system. Best data-fit.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 PAT/PIL Azomethane-Ethene flash-photolysis. Gas-chromatography. Limiting high-pressure k. M = Ar, or SF ₆ . P = (50-1000) torr.	EX	300	(9.03±4.22)(13)			2	
80 SWO/HOC H ₂ O flash-photolysis. P ~760 torr. M = N ₂ , H ₂ .	EX	296	(1.2±0.3)(14)			2	
74 PRA/VEL M = He. M-efficiencies relative to He are: 1.00(He), 37.74(NO).	EX	295	(5.3±1.0)(18)			3	
76 FRA/VEL1 M = He. The preexponential factor expressed as: A(T/298) ^{-0.33} .	EX	321-521	1.06(19)	-0.33	0	3	5.01
H + CH₄ → H₂ + CH₃							
Hydrogen atom + Methane							
71 BAK/BAL Rate constant per CH bond.	CO	298-753	3.1(13)	0	5989	2	
73 CLA/DOV1 BEBO calculation. The preexponential factor expressed as: A(T/298) ^{3.0} .	CO	300-1800	5.93(11)	3.0	4404±20	2	1.05
73 PEE/MAH1	EX	1600	(3.2±0.6)(12)			2	
75 ROT/JUS	EX	1700-2300	7.23(14)	0	7578	2	
78 SHA The preexponential factor expressed as: A(T/298) ² .	CO	300-2500	1.25(12)	2.0	4449	2	
79 SEP/MAR ¹⁾ P(CH ₄) = (17-346) mtorr. P(Ar) = (5.2-14.8) torr.	EX	640-818	1.822(14)	0	6628±421	2	1.82
79 SEP/MAR ¹⁾ Extended T-range by combining the data of several workers. Recommended by author.	RE	400-1800	7.59(13)	0	6002±96	2	1.15
¹⁾ Discharge-flow system.							
80 ROT CH ₄ thermolysis behind shock-waves. Atomic Reso- nance-Absorption. Same data given in 79 ROT/JUS1.	EX	1800-2300	7.23(14)	0	7600	2	
80 MUR/BOR1 ²⁾	RL	1550	8.0(-1)			2/2	
80 MUR/BOR1 ²⁾	RL	1923	1.46			2/2	
²⁾ Oxidative pyrolysis of CH ₄ behind reflected shock-waves, initiated by the N ₂ O decomposition. Within the T-range (1550-1923) K, the ratio of rate constants shows a trend to increase from about 0.7 to 1.5. k _{ref} : N ₂ O + M → N ₂ + O + M.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
D + CD₄ → D₂ + CD₃						
Deuterium atom + Methane-d ₄						
80 CHI/BAK CD ₄ Pyrolysis behind shock-waves. Resonance-absorption Spectroscopy.	EX	1780-2440	2.1(15)	0	11223	2
H + CHO → H₂ + CO (a) → HCHO (b) → O + CH ₂ (c)						
Hydrogen atom + Methyl, oxo-						
73 MAC/THR k _a /k _{ref} . k _{ref} : CHO + O → CO + OH (m) → CO ₂ + H (n)	RL	300	4.0			2/2
78 REI/CLA k _a . HCHO photolysis with tunable pulsed UV laser.	EX	298	3.31(14)			2 2.0
79 NAD/SAR4 k _a . Intracavity laser spectroscopy. Unreported T assumed to be 298 K. Lower-limit k.	EX	298	>3.01(13)			2
81 CHE/RHO k _a . Kinetic modelling of CO oxidation in flames.	ES	250-2000	(4.0±1.0)(13)			2
78 NAD/SAR ¹⁾ k(a + b)/k _{ref} . k _{ref} : CHO + CHO → products.	RL	298	(6.7±2.7)			2/2
78 NAD/SAR ¹⁾ k(a + b).	RN	298	1.45(14)			2
¹⁾ HCHO Flash-photolysis. Laser-spectroscopy.						
79 NAD/SAR2 k _a + k _b . Pulse-photolysis of CH ₃ CHO.	EX	298	(1.20±0.42)(14)			2
80 HOC/SWO1 k _a + k _b . H ₂ flash-photolysis in presence of CO. P = 760 torr.	EX	298	(6.9±1.7)(13)			2
81 TSU/KAT ²⁾ Total conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	RN	1500-1900	1.28(10)	0	-2285	2
81 TSU/KAT ²⁾ Total conc. = 3.0x10 ¹⁹ molec.cm ⁻³ .	RN	1500-1900	4.68(10)	0	-2285	2
81 TSU/KAT ²⁾ Total conc. = 6.0x10 ¹⁹ molec.cm ⁻³ .	DE	1500-1900	6.61(10)	0	-2285	2
²⁾ k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ in Ar behind reflected shock-waves. UV-absorption. IR-emission. k ₁ ~ k ₋₁ K.						
81 TSU/HAS k _c . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ in Ar behind reflected shock-waves.	ES	1200-1800	3.98(13)	0	51602	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + HCHO → H₂ + CHO (a)						
→ CH₂OH (b)						
Hydrogen atom + Formaldehyde						
72 RID/DAV k _a .	EX	297	(3.25±0.30)(10)			2
72 WES/DEH2 k _a .	EX	297-652	1.35(13)	0	1892	2
77 SLE/WAR k _a .	EX	298	(2.59±1.81)(10)			2
78 NAD/SAR k _a . HCHO Flash-photolysis. Laser-spectroscopy.	EX	298	(1.81±0.78)(10)			2
79 KLE k _a . Flash-photolysis. Resonance-fluorescence. Mass-spectrometry.	EX	250-500	(1.97±0.97)(13)	0	1847±184	2
80 DEA/JOH1 k _a . HCHO Decomposition behind shock-waves. Best data-fit. Total conc. = 5x10 ¹⁸ molec.cm ⁻³ .	EX	1700-2500	3.31(14)	0	5281	2
81 TSU/KAT ¹⁾ Total conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	ES	1200-1800	2.95(9)	0	601	2
81 TSU/KAT ¹⁾ Total conc. = 3.0x10 ¹⁹ molec.cm ⁻³ .	ES	1200-1800	1.26(10)	0	601	2
81 TSU/KAT ¹⁾ Total conc. = 6.0x10 ¹⁹ molec.cm ⁻³ .	DE	1200-1800	2.34(10)	0	601	2
¹⁾ k _b . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures diluted in Ar behind reflected shock- waves. UV-absorption. IR-emission. k ₁ = Kk ₋₁ . Same data given in 81 TSU/HAS.						
H + CH₃O → H₂ + HCHO (a)						
→ OH + CH₃ (b)						
Hydrogen atom + Methoxy						
77 MOO/SLE k _a /(k _a + k _b). Most probable ratio.	RL	223-398	(3.1±3.0)(-1)			2/2
77 MOO/SLE k _b /(k _a + k _b). Most probable ratio.	RL	223-398	(6.9±3.0)(-1)			2/2
81 HOY/LOF ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : H + CH ₂ OH → products.	RL	300	6.7(-1)			2/2
81 HOY/LOF ¹⁾ k _a + k _b .	RN	300	2.0(13)			2
¹⁾ Discharge-flow. Laval nozzle. Mass-spectrometry. Channel (a) the major path. P = (0.1-2.0) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + CD₃O → HD + HCHO (a)						
→ OH + CD₃ (b)						
Hydrogen atom + Methoxy-d ₃						
81 HOY/LOF ¹⁾	RL	300	(6.8±1.9)(-1)			2/2
(k _a + k _b)/k _{ref} . k _{ref} : H + CD ₂ OH → products.						
81 HOY/LOF ¹⁾	RN	300	1.9(13)			2
k _a + k _b .						
¹⁾ Discharge fast flow-reactor. Laval nozzle reactor. Mass-spectrometry. Channel (a) is the major path.						
P = (0.1-2.0) torr.						
D + CH₃O → HD + HCHO (a)						
→ OD + CH₃ (b)						
Deuterium atom + Methoxy						
81 HOY/LOF ¹⁾	RL	300	7.1(-1)			2/2
(k _a + k _b)/k _{ref} . k _{ref} : D + CH ₂ OD → products.						
81 HOY/LOF ¹⁾	RN	300	2.2(13)			2
k _a + k _b .						
¹⁾ Discharge fast flow-reactor. Laval nozzle reactor. Mass-spectrometry. Channel (a) is the major path.						
P = (0.1-2.0) torr.						
H + CH₂OH → H₂ + HCHO (a)						
→ OH + CH₃ (b)						
Hydrogen atom + Methyl, hydroxy-						
81 HOY/LOF	RN	300	3.0(13)			2
k _a + k _b . Discharge fast-flow reactor. Laval nozzle reactor. Mass-spectrometry. Channel (a) is the major path.						
P = (0.1-2.0) torr.						
H + CD₂OH → H₂ + DCDO (a)						
→ HD + HCDO (b)						
→ OH + CD₂H (c)						
Hydrogen atom + Methyl-d ₂ , hydroxy-						
81 HOY/LOF	RN	300	2.9(13)			2
k _a + k _b + k _c .						
Discharge fast flow-reactor.						
Laval nozzle reactor. Mass-spectrometry.						
Channels (a) and (b) are major.						
P = (0.1-2.0) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
D + CH ₂ OD → D ₂ + HCHO (a) → DH + HCDO (b) → OD + CH ₂ D (c)						
Deuterium atom + Methyl, hydroxy-d						
81 HOY/LOF k _a + k _b + k _c . Discharge fast flow-reactor. Laval Laval nozzle reactor. Mass-spectrometry. Channels (a) and (b) are major. P = (0.1-2.0) torr.	RN	300	3.2(13)			2
H + CH ₃ OH → H ₂ O + CH ₃ (a) → H ₂ + CH ₂ OH (b) → OH + CH ₄ (c) → H ₂ + CH ₃ O (d)						
Hydrogen atom + Methanol						
71 ADE/WAG k _a + k _b + k _c + k _d .	EX	295-653	(2.3±0.2)(13)	0	2667±151	2
73 ADE k _a + k _b .	EX	298-650	1.3(13)	0	2670	2
74 MEA/KIM k _b . Flow-discharge method with ESR detection.	EX	298-565	(1.80±0.33)(12)	0	2738±65	2
74 MEA/KIM k _b . Assumed A-factor on the basis of stoichiometric considerations. Recommended k.	RE	298-575	6.5(12)	0	2738±75	2
81 HOY/SIE k _b + k _d . Isothermal discharge-flow reactor. Mass-spectrometry. P = (1.5-6) torr.	EX	500-680	1.3(13)	0	2646	2
81 VAN/VAN k _b . Methanol oxidation in lean flames. CH ₃ OH/O ₂ mixtures, with or without added Ar or H ₂ , burned at 40 torr. Molecular beam sampling. Mass-spectrometry.	DE	1000-2000	3.4(13)	0	1309	2
H + CD ₃ OH → H ₂ + CD ₃ O (a) → HD + CD ₂ OH (b)						
Hydrogen atom + Methan-d ₃ -ol						
81 HOY/SIE k _a + k _b . Isothermal discharge-flow reactor. Mass-spectrometry. P = (1.5-6) torr.	EX	500-680	1.3(13)	0	2646	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + CD₃OD → HD + CD₃O (a)						
→ HD + CD₂OD (b)						
Hydrogen atom + Methanol-d ₄						
81 HOY/SIE	EX	500-680	1.3(13)	0	2646	2
k _a + k _b . Discharge-flow. P = (1.5-6) torr.						
D + CH₃OH → DH + CH₃O (a)						
→ DH + CH₂OH (b)						
Deuterium atom + Methanol						
81 HOY/SIE	EX	500-680	1.3(13)	0	2646	2
k _a + k _b . Discharge-flow. P = (1.5-6) torr.						
74 MEA/KIM	ES	298-575	(2.82±0.40)(13)	0	2617±50	2
k _b . Discharge-flow with ESR detection.						
H + CH₃OOH → H₂O + CH₃O (a)						
→ H₂ + CH₃O₂ (b)						
→ H₂ + CH₂OOH (c)						
Hydrogen atom + Hydroperoxide, methyl-						
75 SLE/WAR2	EX	250-358	(1.69±0.54)(11)	0	956±101	2
k _a + k _b + k _c .						
77 SLE/WAR	EX	250-358	(7.27±0.18)(10)	0	936±96	2
k _a = (43±7)% of k(overall).						
77 SLE/WAR	EX	250-358	(8.79±0.18)(10)	0	936±96	2
k _b = (52±7)% of k(overall).						
77 SLE/WAR	EX	250-358	8.45(9)	0	936±96	2
k _c = 5% of k(overall).						
77 SLE/WAR ¹⁾	EX	250-358	(1.69±0.54)(11)	0	936±96	2
77 SLE/WAR ¹⁾	EX	298	(7.83±1.20)(9)			2
¹⁾ k _a + k _b + k _c .						
D + CH₃OOH → DHO + CH₃O (a)						
→ DH + CH₃O₂ (b)						
→ DH + CH₂OOH (c)						
Deuterium atom + Hydroperoxide, methyl-						
77 SLE/WAR	EX	298	(7.23±0.60)(9)			2
k _a + k _b + k _c .						
H + COS → SH + CO						
Hydrogen atom + Carbon oxide sulfide						
72 ROM/SCH	EX	298	(1.33±0.24)(10)			2
75 TSU/YOK	EX	300-525	(9.1±1.2)(12)	0	1963±186	2
76 LEE	EX	298-478	(9.77±1.00)(13)	0	2774±39	2
77 LEE/STI	EX	261-500	(5.46±0.92)(12)	0	1938±55	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	E, B-B(ref)	k,A units	k err. factor
$H + CH_2=N=N \rightarrow CH_3 + N_2$ Hydrogen atom + Methane, diazo-	EX	300	9.64(12)				2
72 NIK/MOR2							
$H + CH_3NO_2 \rightarrow$ products Hydrogen atom + Methane, nitro-	EX	298-398	(1.63±0.60)(12)	0	1761±126		2
75 SLE/WAR2							
$H + CH_3ONO \rightarrow NO + CH_3OH$ (a) → $H_2 + CH_2ONO$ (b) → $HNO + CH_3O$ (c) Hydrogen atom + Nitrous acid methyl ester (Methyl nitrite)	EX	223-398	(1.21±0.13)(11)	0	956±55		2
77 MOO/SLE $k_a = (47±5)\%$ of k(overall).							
77 MOO/SLE $k_b + k_c = (53±5)\%$ of k(overall).	EX	223-398	(1.37±0.13)(11)	0	956±55		2
77 MOO/SLE $k_a + k_b + k_c$.	EX	223-398	(2.58±0.51)(11)	0	956±55		2
$H + CD_3ONO \rightarrow NO + CD_3OH$ (a) → $HD + CH_2ONO$ (b) → $HNO + CD_3O$ (c) Hydrogen atom + Nitrous acid methyl-d ₃ ester (Methyl-d ₃ nitrite)	EX	298	(8.31±1.39)(9)				2
77 MOO/SLE $k_a + k_b + k_c$.							
$H + CH=CH (+ M) \rightarrow H_2 + CH=C (+ M)$ (a) → $CH_2=CH (+ M)$ (b) Hydrogen atom + Ethyne	EX	1063-1233	4.78(13)	0	8254±2013		2.51
74 YAM/LAV k_a .							
71 OSB ¹⁾	EX	298	2.71(10)				2
75 IBU/TAK ¹⁾ ¹⁾ k_b .	EX	296	(5.5±0.5)(10)				2
76 KEI/LYN ²⁾ k increasing from $(6.32±0.60) \times 10^9$ to $(1.29±0.12) \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ within the (1-10) torr. P=range. Low P-range. $k_b = k_{app}/s$, where $s \sim 2.0$.	EX	298	(6.32±0.60)(9)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err. factor
76 KEI/LYN ²) k increasing from $(2.37 \pm 0.26) \times 10^{10}$ to $(9.43 \pm 0.58) \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ within the (6-742) torr. P-range. High P-range. $k_{bi} = k_{app}/s$, where $s \sim 1.15$.	EX	298	$(2.37 \pm 0.86)(10)$				2
²) k_p . Initial step in a proposed mechanism. Addition product vibrationally excited. P-dependent k's.							
76 PAY/STI k_p . M = He. Limiting high-pressure k. Initial step in a proposed mechanism.	EX	193-400	$(5.54 \pm 1.57)(12)$	0	1213 ± 70		2
78 GOR/IVA2 ³) Method based on collision-induced shifts and HF-transition line broadening in H atoms.	EX	305	$(2.11 \pm 0.18)(11)$				2
78 GOR/IVA2 ³) Method based on H-maser relaxation.	EX	305	$(2.11 \pm 0.12)(11)$				2
78 GOR/IVA2 ³) Method based on collision-induced shifts and HF-transition line broadening in H atoms.	EX	305	$(9.43 \pm 3.63)(16)$				3
³) k_p .							
79 ISH/SUG2 k_p . Pulse-radiolysis. Absorption-Spectroscopy. P = (200-1100) torr. H + 0.073 torr. CH=CH.	EX	298	$(2.28 \pm 0.24)(11)$				2
81 SUG/OKA2 k_p . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k.	EX	206-461	$(2.28 \pm 0.12)(13)$	0	1374 ± 18		2
H + CD=CD (+ M) → D + CH=CD (+ M) (a) → CHD=CD (+ M) (b)							
Hydrogen atom + Ethyne-d ₂							
71 HOY/WAG k_a .	EX	300-470	2.0(13)	0	2667 ± 252		2
76 KEI/LYN ¹) k increasing from $(3.98 \pm 0.42) \times 10^{10}$ to $(5.84 \pm 0.60) \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ within the (1.2-5.6) torr. pressure range. Experiments in excess [CD=CD].	EX	298	$(3.98 \pm 0.42)(10)$				2
76 KEI/LYN ¹) k increasing from $(2.11 \pm 0.24) \times 10^{10}$ to $(3.49 \pm 0.36) \times 10^{10} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ within the (1-5) torr. pressure range. Experiments in excess [H].	EX	298	$(2.11 \pm 0.24)(10)$				2
¹) k_a . Overall reaction of a proposed mechanism. P-dependent rate constants.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 GOR/IVA2 ²)	EX	305	(2.35±0.48)(11)			2	
78 GOR/IVA2 ²)	EX	305	(9.98±5.44)(16)			3	
²) k _b . Collision-induced shifts. HF-transition line broadening in H atoms.							
79 ISH/SUG2	EX	298	(2.29±0.12)(11)			2	
k _b . Pulse-radiolysis. Absorption-spectroscopy. P = (200-1100) torr. (H ₂ + CD≡CD)							
81 SUG/OKA2	EX	206-461	(1.91±0.12)(13)	0	1330±24	2	
k _b . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k.							
D + CH≡CH → H + CH=CD (a) → CHD=CH (b)							
Deuterium atom + Ethyne							
71 HOY/WAG	EX	200-465	3.1(13)	0	1862±101	2	
k _a .							
76 KEI/LYN	EX	298	(7.35±0.72)(10)			2	
k _a . Overall reaction of a proposed mechanism. Average k for the pressure range (1-6.7) torr.							
79 ISH/SUG2	EX	298	(1.57±0.12)(11)			2	
k _b . Pulse-radiolysis. Absorption-spectroscopy. P = (200-1100) torr. (D ₂ + CH≡CH)							
81 SUG/OKA2	EX	206-461	(2.07±0.37)(13)	0	1521±59	2	
k _b . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k.							
D + CD≡CD → CD ₂ =CD							
Deuterium atom + Ethyne-d ₂							
76 KEI/LYN	EX	298	(6.63±0.60)(9)			2	
k increasing from (6.63±0.60)×10 ⁹ to (1.08±0.12)×10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ within the (1-5 6) torr. P-range. P-dependent k. k _{bi} = k _{app} /s, where s ~ 2.0. The addition product is vibrationally excited.							
79 ISH/SUG2	EX	298	(1.51±0.12)(11)			2	
Pulse-radiolysis. Absorption-spectroscopy. P = (200-1100) torr. (D ₂ + CD≡CD)							
81 SUG/OKA2	EX	206-461	(2.64±0.87)(13)	0	1602±18	2	
Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + CH₂=CH → H₂ + CH=CH						
Hydrogen atom + Ethenyl						
80 TAN/GAR1 Thermolysis of CH ₂ =CH ₂ in Ar behind incident shock-waves. Optimization. Total conc. = (1.1-2.2)x10 ¹⁸ molec.cm ⁻³ .	ES	2000-2450	1.0(13)	0	0	2
H + CH₂=CH₂ (+ M) → H₂ + CH₂=CH (+ M) (a) → CH₃CH₂ (+ M) (b)						
Hydrogen atom + Ethene						
72 FAL/SUN k _a /k _b . Upper-limit ratio.	RL	298	≤3.0(-4)			2/2
73 PEE/MAH2 ¹⁾	ES	1200-1700	1.1(14)	0	4278	2
74 YAM2 ¹⁾	EX	1093-1213	1.91(13)	0	5184±1007	2 2.51
75 NAM/SHE ¹⁾	EX	1073-1173	(1.5±0.4)(11)			2
75 NAM/SHE ¹⁾ A-factor recalculated from the author's estimated value for E _a .	ES	1073-1173	8.47(12)	0	4529±201	2
77 JUS/ROT ¹⁾	ES	1700	5.0(12)			2
77 JUS/ROT ¹⁾	ES	2000	1.5(13)			2
77 JUS/ROT ¹⁾	ES	1700-2000	5.0(15)	0	11500	2
81 HAU/SAN ¹⁾ Propane pyrolysis. Adiabatic flow-reactor.	EX	1110-1235	3.54(14)	0	7217	2
¹⁾ k _a .						
71 COW/KEI ²⁾ k _b /k _{ref} . k _{ref} : H + CH=CH → CH ₂ =CH [†]	RL	298	(8.6±1.3)			2/2
71 COW/KEI ²⁾ k _b .	RN	298	(2.35±0.60)(11)			2
²⁾ M = Ne, Ar. Steady-state photolysis method. The addition product is vibrationally excited. P(Total) = (10-15) torr.						
71 HIK/EYR k _b . M = H ₂ , or Ar. Limiting high-pressure k. The addition product is vibrationally excited.	EX	298	(5.5±0.5)(11)			2
71 OSB k _b .	EX	298	3.70(11)			2
71 PEN/DAR ³⁾ k _b /k _{ref} . k _{ref} : H + HI → H ₂ + I.	RL	303-478	3.0(-1)	0	425	2/2
71 PEN/DAR ³⁾ k _b .	RN	298	(6.9±0.7)(11)			2
³⁾ Photolysis of HI in presence of Ethene.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 TEN/JON k_b . Data-fit to a proposed mechanism.	CO	303-603	7.89(11)	0	367	2
73 MIC/OSB k_b . M = He. Limiting high-pressure k.	EX	298	(9.70±0.19)(11)			2
74 LAU/BUE ⁴⁾ k_{ref} : H + CH ₃ CH=CH ₂ → (CH ₃) ₂ CH [†]	RL	298	(5.6±0.2)(-1)			2/2
74 LAU/BUE ⁴⁾ k_{ref} : H + CH ₃ CH=CHCH ₃ → CH ₃ CH ₂ CHCH ₃ [†]	RL	298	(1.2±0.2)			2/2
74 LAU/BUE ⁴⁾ k_{ref} : H + (CH ₃) ₂ C=CHCH ₃ → (CH ₃) ₂ CCH ₂ CH ₃ [†] (c) → (CH ₃) ₂ CHCHCH ₃ [†] (d)	RL	298	(8.0±2.0)(-1)			2/2
⁴⁾ k_b/k_{ref} . The product is vibrationally excited.						
74 LAU/BUE k_b . The product is vibrationally excited.	EX	298	2.47(11)			2
75 IBU/TAK k_b/k_{ref} . Conventional vacuum apparatus. k_{ref} : H + CH≡CH → CH ₂ =CH	RL	296	9.99±0.16			2/2
75 MIH/SCH k_b . The product is vibrationally excited.	EX	295	(7.53±0.24)(11)			2
78 GOR/IVA2 k_b . Method based on collision-induced shifts and HF-transition line broadening in H atoms.	EX	305	(6.32±0.60)(11)			2
78 GOR/IVA2 k_b . Method based on H-maser relaxation.	EX	305	(6.63±0.12)(11)			2
78 GOR/IVA2 k_b . Method based on collision-induced shifts and HF-transition line broadening in H atoms.	EX	305	(4.35±1.45)(17)			3
78 ISH/YAM k_b . Pulse-radiolysis. Resonance-absorption. P(H ₂) = (200-1200) torr.	EX	298	(6.63±0.60)(11)			2
78 LEE/MIC1 k_b . M = Ar. Flash-photolysis. Resonance-fluorescence. P(CH ₂ =CH ₂) = (13-150) torr. P(Ar) = (300-760) torr.	EX	198-320	(2.21±0.40)(13)	0	1040±42	2
79 OKA/CVE ⁵⁾ k_b/k_{ref} . k_{ref} : H + NO + M → HNO + M.	RL	298	(3.41±0.06)(-2)			2/3
79 OKA/CVE ⁵⁾ k_b .	RN	298	(4.69±0.15)(11)			2
⁵⁾ Modulated Hg-photosensitization. Chemiluminescence. k is P-dependent, decreasing with lower P-values. The product is vibrationally excited. P = 100 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 BIL/BAR k_b . Ethane pyrolysis. k determined relative to the reaction: $H + CH_3CH_3 \rightarrow H_2 + CH_3CH_2$	RN	793-829	3.98(13)	0	2345	2	
81 EKW/SAF2 k_b/k_{ref} . H atoms generated by Hg-photosensitized decomposition of H_2 . General vacuum apparatus. Gas-chromatography. $P(H_2) \sim 580$ torr. $P(\text{Diethylsulfide}) = (1-32)$ torr. k_{ref} : $H + (CH_3CH_2)_2S \rightarrow CH_3CH_2SH + CH_3CH_2$	RL	358-461	4.66(-1)	0	-871±35	2/2	
81 SUG/OKA2 k_b . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.83±0.30)(13)	0	1096±29	2	
$H + CH_2=CHD \rightarrow CH_3CHD$ (a)							
$\rightarrow CH_2DCH_2$ (b)							
Hydrogen atom + Ethene-d							
81 SUG/OKA2 $k_a + k_b$. Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.67±0.46)(13)	0	1084±50	2	
$H + CD_2=CD_2 (+ M) \rightarrow D + CD_2=CDH (+ M)$ (a)							
$\rightarrow CD_2HCD_2 (+ M)$ (b)							
Hydrogen atom + Ethene-d ₄							
74 YAM1 k_a . Averaged over the given T-range.	EX	1000-1200	6.75(12)			2	1.35
71 OSB k_b .	EX	298	5.44(11)			2	
71 PEN/DAR ¹⁾ k_b/k_{ref} . k_{ref} : $H + HI \rightarrow H_2 + I$.	RL	303-478	3.0(-1)	0	425	2/2	
71 PEN/DAR ¹⁾ k_b .	RN	298	(7.6±0.8)(11)			2	
¹⁾ Photolysis of HI in presence of $CD_2=CD_2$.							
75 COW/MIC k_b . In excess H, at 0.91rr. k increasing to $5.90 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 4.93 torr.	EX	297	4.16(11)			2	
75 MIH/SCH k_b . The product is vibrationally excited.	EX	295	(6.93±0.24)(11)			2	
78 GOR/IVA2 k_b . Collision-induced shifts. HF-transition line broadening in H atoms.	EX	305	(6.99±0.48)(11)			2	
78 GOR/IVA2 k_b . Method based on H-maser relaxation.	EX	305	(6.02±0.12)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 GOR/IVA2 k_b . Collision-induced shifts. HF-transition line broadening in H atoms.	EX	305	(3.63±1.09)(17)				3
81 SUG/OKA2 k_b . Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.75±0.30)(13)	0	1087±26		2
+ $\text{CH}_2=\text{CH}_2 \rightarrow \text{CDH}_2\text{CH}_2$							
Deuterium atom + Ethene							
75 COW/MIC In excess D. P-independent from 0.96 to 5 torr.	EX	297	(4.60±0.04)(11)				2
75 COW/MIC In excess $\text{CH}_2=\text{CH}_2$. Relatively stable k from 1.25 to 1.76 torr., but increasing to $7.29 \times 10^{11} \text{ cm}_3 \text{ mol}^{-1} \text{ a}^{-1}$ at 4.16 torr.	EX	297	(4.68±0.34)(11)				2
75 MIH/SCH The product is vibrationally excited.	EX	295	(5.24±0.18)(11)				2
79 ISH/SAT Pulse-radiolysis. Resonance-absorption.	EX	298	(4.82±0.60)(11)				2
81 SUG/OKA2 Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.02±0.09)(13)	0	1100±12		2
D + $\text{CH}_2=\text{CHD} \rightarrow \text{CDH}_2\text{CHD}$ (a) $\rightarrow \text{CD}_2\text{HCH}_2$ (b)							
Deuterium atom + Ethene-d							
81 SUG/OKA2 $k_a + k_b$. Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.15±0.20)(13)	0	1104±28		2
D + $\text{CD}_2=\text{CD}_2 \rightarrow \text{CD}_3\text{CD}_2$							
Deuterium atom + Ethene-d ₄							
71 OSB	EX	298	4.37(11)				2
75 COW/MIC In excess D, at 0.95 torr. k increasing to $2.77 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ at 5 torr.	EX	297	1.33(11)				2
75 MIH/SCH The product is vibrationally excited.	EX	295	(5.12±0.30)(11)				2
81 SUG/OKA2 Pulse-radiolysis. Resonance-absorption. Limiting high-pressure k. Supersedes 81 SUG/OKA1.	EX	206-461	(2.14±0.26)(13)	0	1115±36		2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + CH₃CH₂ → CH₃ + CH₃ (a)						
→ H₂ + CH₂=CH₂ (b)						
Hydrogen atom + Ethyl						
72 TEN/JON ¹⁾	DE	303-603	1.08(14)	0	438	2
Data-fit to a proposed mechanism.						
74 CAM/MAR ¹⁾	EX	503-753	3.72(13)	0	0	2
74 PRA/VEL ¹⁾	EX	295	(4.3±0.4)(13)			2
76 PRA/VEL1 ¹⁾	EX	321-521	6.46(13)	0	112±35	2 1.12
79 TAB/BAU ¹⁾	EX	1950-2770	1.0(13)	0	0	2
M = Ar. CH ₄ pyrolysis in shock-waves.						
Best data-fit.						
Total conc. = (1.4-5.4)x10 ¹⁸ molec.cm ⁻³ .						
¹⁾ k _a .						
74 CAM/MAR	EX	503-753	1.70(12)	0	0	2
k _b .						
H + CH₃CH₃ → H₂ + CH₃CH₂						
Hydrogen atom + Ethane						
71 BAK/BAL	CO	298-753	2.2(13)	0	4882	2
Rate constant per CH bond.						
72 KAL/KOR	ES	1073-1173	(3.31±2.71)(12)	0	0	2
Average of two given values.						
73 CLA/DOV1	CO	300-1800	2.45(11)	3.5	2617±35	2 1.07
BEBO calculation. The preexponential factor expressed as: A(T/298) ^{3.5} .						
74 CAM/MAR	SE	290-1290	1.32(14)	0	4715±108	2 1.23
74 CAM/MAR	EX	503-753	1.86(14)	0	4920±192	2 1.35
74 KAL/SHE	EX	1023-1123	(2.4±0.6)(12)			2
77 JON/MOR	EX	357-544	1.07(14)	0	4642±313	2 1.86
Discharge-flow. Mass-spectrotry.						
78 LED/VIL	EX	281-1485	5.01(13)	0	4580±302	2 3.98
Discharge-flow reactor.						
79 BAL/WAL1	CO	753-773	1.32(14)	0	4715	2
A and B recalculated from an empirical formula.						
H + CH₂=C=O → CH₃ + CO						
Hydrogen atom + Ethenone (Ketene)						
75 SLE/WAR1	EX	218-363	(3.61±1.20)(12)	0	1178±101	2
75 SLE/WAR1	EX	300	(7.23±0.60)(10)			2
79 MIC/NAV1 ¹⁾	EX	298-500	(1.13±0.67)(13)	0	1725±190	2
79 MIC/NAV1 ¹⁾	EX	298	(3.73±1.01)(10)			2
79 MIC/NAV1 ¹⁾	EX	298	(4.40±0.78)(10)			2
¹⁾ Flash-photolysis. Discharge-flow.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$H + CH_3CO \rightarrow H_2 + CH_2=C=O$ (a) $\rightarrow CHO + CH_3$ (b)							
Ethyl, 1-oxo- + Hydrogen atom							
75 SLE/WAR1 $k_a/(k_a + k_b)$.	RL	298	(6.3±0.7)(-1)				2/2
75 SLE/WAR1 $k_b/(k_a + k_b)$.	RL	298	3.7(-1)				2/2
$H + CH_3CHO \rightarrow H_2 + CH_3CO$							
Hydrogen atom + Acetaldehyde							
73 ADE/WAG1	EX	295-389	(2.6±0.2)	0	1309±75		2
75 SLE/WAR1 $k_{ref}: H + CH_2=C=O \rightarrow CO + CH_3$	RL	298	(4.6±0.2)(-1)				2/2
75 SLE/WAR1	RN	298	3.19(10)				2
76 WHY/MIC2	EX	298-500	(1.34±0.23)(13)	0	1661±60		2
77 MIC/LEE Discharge-flow. Resonance-fluorescence.	EX	298	(5.90±0.48)(10)				2
$H + CH_2CH_2OH \rightarrow H + [C_2H_4O]$							
Hydrogen atom + Ethyl, 2-hydroxy-							
82 BAR/HOY Discharge-flow. Laval-nozzle. P < 0.2 torr.	EX	~295	≈5.0(13)				2
$H + CH_3CH_2OH \rightarrow H_2 + CH_3CHOH$ (a) $\rightarrow H_2O + CH_3CH_2$ (b)							
Hydrogen atom + Ethanol							
73 ADE/WAG2 k_a .	EX	295-700	≈4.4(12)	0	2300		2
73 ADE/WAG2 k_b .	EX	295-700	≈5.9(11)	0	1736		2
73 ADE ¹⁾	EX	298-470	4.2(12)	0	2117		2
73 ADE/WAG2 ¹⁾ ¹⁾ $k_a + k_b$.	EX	295-700	(4.2±0.4)(12)	0	2115±150		2
$H + (CH_3)_2O \rightarrow H_2 + CH_3OCH_2$							
Hydrogen atom + Methane, oxybis-							
74 MEA/KIM ¹⁾ Electron-Spin-Resonance measurements.	EX	300-404	(2.61±0.13)(13)	0	2365±25		2
74 MEA/KIM ¹⁾ Mass-spectrometric measurements, assumed free from stoichiometric factors.	EX	300-404	(1.3±0.5)	0	2365±50		2
¹⁾ Flow-discharge method.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 SLE/WAR	EX	298	(7.83±2.41)(8)			2	
78 ARO ²⁾	ES	1062	2.0(12)			2	
78 ARO ²⁾	ES	1223	2.0(13)			2	
²⁾ Pyrolysis in a flow-reactor.							
78 LEE/MAC	EX	273-426	(2.64±0.36)(12)	0	1956±43	2	
Flash-photolysis. Resonance-fluorescence.							
79 FAU/HOY	EX	250-620	(1.9±0.9)(13)	0	2600±100	2	
Discharge-flow. Mass-spectrometry.							
81 LEE/MAC	EX	273-426	(2.64±0.36)(12)	0	1956±43	2	
Flash-photolysis. Resonance-fluorescence.							
[(CH ₃) ₂ O] ₀ ~1.0x10 ¹⁶ molec.cm ⁻³ .							
[H] ₀ <1.0x10 ¹¹ molec.cm ⁻³ .							
D + (CH₃)₂O → DH + CH₃OCH₂							
Deuterium atom + Methane, oxybis-							
74 MEA/KIM	EX	198-363	(4.14±0.73)(13)	0	2229±50	2	
Flow-discharge method with ESR detection.							
H + CH₃OOCH₃ → H₂ + CH₂OOCH₃							
Hydrogen atom + Peroxide, dimethyl-							
77 SLE/WAR	EX	298	(7.23±0.60)(8)			2	
H + \triangle → SH + CH₂=CH₂							
Hydrogen atom + Thiirane (Ethylene episulfide)							
75 YOK/AHM	RN	300-425	(5.7±0.7)(13)	0	978±88	2	
76 LEE	EX	298	(7.10±1.08)(11)			2	
77 LEE/STI	EX	223-423	(1.73±0.07)(13)	0	946±12	2	
H + (CH₃)₂S → H₂ + CH₃SCH₂ (a)							
→ CH₃ + CH₃SH (b)							
Hydrogen atom + Methane, thiobis-							
76 LEE	EX	300	(9.0±3.0)(10)			2	
k _a + k _b .							
81 LEE/MAC ¹⁾	EX	212-500	(7.83±2.59)(12)	0	1118±81	2	
81 LEE/MAC ¹⁾	EX	212-298	(2.60±0.36)(12)	0	853±23	2	
81 LEE/MAC ¹⁾	EX	298-500	(1.51±0.04)(13)	0	1372±9	2	
¹⁾ k _a . Flash-photolysis.							
Resonance-fluorescence. Gas-chromatography.							
Arrhenius plot seems curved over the whole							
whole T-range of (212-500) K.							
[(CH ₃) ₂ S] ₀ ~1.0x10 ¹⁴ molec.cm ⁻³ .							
[H] ₀ <1.0x10 ¹¹ molec.cm ⁻³ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 YOK/STR k _b . H atoms generated by H ₂ S photolysis in excess He, or CO ₂ . General-vacuum system. P = 760 torr.	EX	300-472	(1.71±0.26)(13)	0	1319±44	2
H + CH ₃ SSCH ₃ → CH ₃ SH + CH ₃ S Hydrogen atom + Disulfide, dimethyl-						
80 EKW/JOD Hg-sensitized reaction. P(H ₂) = (570-590) torr.	EX	298-428	(5.7±1.2)(12)	0	50±50	2
H + NCCN → HCN + CN (a) → HC ₂ N ₂ [†] (b) Hydrogen atom + Ethanedinitrile						
71 DUN/FRE k _a . P(Total) ~ 1 torr.	EX	298	(5.18±1.81)(8)			2
78 PHI k _b . Discharge-flow. Resonance-fluorescence. High-pressure k.	EX	300	(9.03±1.20)(8)			2
H + O=C=C=C=O → CO + OC=CH Hydrogen atom + 1,2-Propadiene-1,3-dione						
77 FAU/WAG1	EX	295-480	(1.7±0.6)(13)	0	1480±180	2
H + CH ₃ C=CH → CH ₃ C=CH ₂ [†] (a) → CH ₃ CH=CH [†] → CH ₃ + CH=CH (b) Hydrogen atom + 1-Propyne						
72 WAG/ZEL2 k _a .	EX	195-503	(6.5±1.2)(12)	0	1007±101	2
72 WAG/ZEL2 k _b .	EX	195-503	(5.8±1.2)(12)	0	1560±126	2
76 WHY/PAY k _a + k _b .	EX	215-460	(3.61±0.72)(13)	0	1233±50	2
77 MIC/LEE k _b . Discharge-flow. Resonance-fluorescence. [H] ₀ ~ 1.0x10 ¹¹ molec.cm ⁻³ . P(He) = 2 torr.	EX	298	(3.79±0.24)(11)			2
H + CH ₂ =C=CH ₂ → CH ₃ C=CH ₂ [†] (a) → CH ₂ CH=CH ₂ [†] (b) Hydrogen atom + 1,2-Propadiene (Allene)						
72 WAG/ZEL3 k _a .	EX	273-470	(8.5±2.0)(12)	0	1007±101	2
72 WAG/ZEL3 k _b .	EX	273-470	(4.0±2.0)(12)	0	1359±201	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 ALE/ARU1 ¹⁾ P = 4.0 torr.	EX	295	1.51(11)			2
80 ALE/ARU1 ¹⁾ P = 3.9 torr.	EX	363	2.89(11)			2
80 ALE/ARU1 ¹⁾ P = 4.0 torr.	EX	523	1.16(12)			2
80 ALE/ARU1 ¹⁾ P = 4.9 torr.	EX	853	1.69(12)			2
¹⁾ k _{overall} . Resonance-fluorescence. k values are given for other, lower pressures.						
H + CH ₃ CH=CH ₂ → H ₂ + CH ₂ =CHCH ₂ (a) → CH ₃ CH ₂ CH ₂ (b) → (CH ₃) ₂ CH (c) → CH ₃ + CH ₂ =CH ₂ (d)						
Hydrogen atom + 1-Propene						
72 FAL/SUN k _a /(k _b + k _c).	RL	298	2.0(-3)			2/2
72 WAG/ZEL1 k _b .	EX	195-390	(4.4±0.6)(12)	0	1384±101	2
78 MAR/PUR k _b /k _{ref} . 2,2,3,3-Tetramethylbutane pyrolysis. Static system. P = (3-19) torr. k _{ref} : H + (CH ₃) ₂ C=CH ₂ → (CH ₃) ₃ C Rate ratio determined on the basis of reaction: (CH ₃) ₃ CC(CH ₃) ₃ → (CH ₃) ₃ C + (CH ₃) ₃ C	RL	718	2.2			2/2
71 COW/KEI ¹⁾ k _b + k _c . M = He. Discharge-flow. k increasing to (4.82±0.48)×10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ for (0.96-4.91) torr.	EX	298	(4.00±0.36)(11)			2
71 COW/KEI ¹⁾ (k _b + k _c)/k _{ref} . M = Ne, Ar. Steady-state photolysis method. P = (10-15) torr. k _{ref} : H + CH≡CH → CH ₂ =CH [†]	RL	298	(2.08±0.09)(1)			2/2
71 COW/KEI ¹⁾ k _b + k _c . M = Ne, Ar. P = (10-15) torr. Steady-state photolysis method.	RN	298	(5.66±0.84)(11)			2
¹⁾ The products of channels (b) and (c) are vibrationally excited.						
71 DAB/NIK k _b + k _c . M = He. P = (1.0-2.4) torr. The products of channels (b) and (c) are vibrationally excited.	EX	298	(4.55±0.26)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 KUR/PET2 $k_b + k_c$. Resonance-fluorescence. The products of (b) and (c) are vibrationally excited. P(Total) = 50 torr.	EX	177-473	(6.13±0.16)(12)	0	609±6	2
75 MIH/SCH $k_b + k_c$. The products of channels (b) and (c) are vibrationally excited.	EX	295	(1.01±0.30)(12)			2
78 ISH/YAM $k_b + k_c$. Pulse-radiolysis. Resonance-absorption. Predominant paths. P(H ₂) = (200-1200) torr.	EX	298	(1.02±0.06)(12)			2
79 OKA/CVE ²) ($k_b + k_c$)/ k_{ref} . k_{ref} : H + NO + M → HNO + M	RL	298	(4.81±0.07)(-2)			2/3
79 OKA/CVE ²) $k_b + k_c$.	RN	298	(8.33±0.16)(11)			2
²) Modulated Hg-photosensitization. Chemiluminescence. The products are vibrationally excited. P = 50 torr.						
82 HAR/PIT $k_b + k_c$. Flash-photolysis. Resonance-fluorescence. H atoms generated by pulsed vacuum-UV Photolysis of CH ₄ . Gas-chromatography. Predominant paths. The products of channels (b) and (c) are vibrationally excited. P(Total) = 50 torr.	EX	298-445	(1.33±0.15)(13)	0	785±54	2
82 WAT/KYO $k_b + k_c$. Pulse-radiolysis. Resonance-absorption. Gas-chromatography. P(H ₂) ~ 500 torr. P(CH ₃ CH=CH ₂) = (0.01-0.1) torr.	EX	200-500	(1.81±0.23)(13)	0	811±33	2
72 WAG/ZEL1 k_c .	EX	195-390	(5.4±0.6)(12)	0	629±50	2
74 LAU/BUE k_c/k_{ref} . k_{ref} : H + CH ₂ =CH ₂ → CH ₃ CH ₂ [†] . The products of channel (c) are vibrationally excited.	RL	298	(1.79±0.04)			2/2
75 CAM/MAR k_c . Determined from k_{-c} and published thermochemical data.	CO	576-813	6.31(12)	0	842	2
71 LEX/MAR1 k_d/k_c . M = Ar. Discharge flow method. The product of channel (c) is vibrationally excited. P(Ar) = (4-16) torr.	RL	290	(4.04±0.29)(-2)			2/2
72 KAL/KOR k_d .	EX	1073-1173	(4.52±0.90)(12)	0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + CD₃CD=CD₂ → CD₃CDECD₂ (a)						
→ CD₃CDCD₂H (b)						
Hydrogen atom + 1-Propene-1,1,2,3,3,3-d ₆						
82 WAT/KYO	EX	200-500	(1.54±0.34)(13)	0	759±64	2
k _a + k _b . Pulse-radiolysis. Resonance-absorption. P(CD ₃ CD=CD ₂) = (0.01-0.1) torr. P(H ₂) ~ 500 torr.						
D + CH₃CH=CH₂ → CH₃CHDCH₂ (a)						
→ CH₃CHCH₂D (b)						
Deuterium atom + 1-Propene						
71 DAB/NIK	EX	298	(6.20±0.66)(11)			2
k _a + k _b . M = He. P = (0.6-2.2) torr. The products of channels (a) and (b) are vibrationally excited.						
75 MIH/SCH	EX	295	(6.87±0.24)(11)			2
k _a + k _b . The products of channels (a) and (b) are vibrationally excited.						
79 ISH/SAT	EX	298	(7.83±1.20)(11)			2
k _a + k _b . Pulse-radiolysis. Resonance-absorption.						
82 WAT/KYO	EX	200-500	(1.20±0.03)(13)	0	780±8	2
k _a + k _b . Pulse-radiolysis. Resonance-absorption. P(CH ₃ CH=CH ₂) = (0.01-0.1) torr. P(D ₂) ~ 500 torr.						
77 YAN	RL	1260-1360	(6.5±1.5)(-1)	0	0	2/2
k _a /k _b . Estimated ratio. Thermolysis of 1-Propene in presence of D ₂ , in Ar, in a single shock-tube. P(D ₂) ~ 500 torr.						
D + CD₃CD=CD₂ → CD₃CD₂CD₂ (a)						
→ (CD₃)₂CD (b)						
Deuterium atom + 1-Propene-1,1,2,3,3,3-d ₆						
82 WAT/KYO	EX	200-500	(1.33±0.16)(13)	0	799±34	2
k _a + k _b . Pulse-radiolysis. Resonance-absorption. P(CD ₃ CD=CD ₂) = (0.01-0.1) torr. P(D ₂) ~ 500 torr.						
H + (CH₃)₂CH → H₂ + CH₃CH=CH₂ (a)						
→ CH₃CH₂CH₃ (b)						
Hydrogen atom + Ethyl, 1-methyl-						
71 LEX/MAR1 ¹	RL	290	(7.19±0.12)(-1)			2/2
k _a /k _b . P(Ar) = (4-16) torr.						
71 LEX/MAR2 ¹	RL	290	(5.4±1.1)(-1)			2/2
k _a /k _b . P(Ar) = (4-12) torr.						
¹) Discharge flow. The product of channel (b) is vibrationally excited.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H + (CH₃)₂CH[†] → CH₃ + CH₃CH₂						
Hydrogen atom + Ethyl, 1-methyl-						
71 LEX/MAR1 Discharge-flow. P(Total) = (4-16) torr. (CH ₃)CH ^{>} assumed to be formed from H + CH ₃ CH=CH ₂ . k _{ref} : (CH ₃) ₂ CH [†] + M → (CH ₃) ₂ CH + M	RL	290	(4.84±0.28)(1)			2/2
H + CH₃CH₂CH₃ → H₂ + CH₃CH₂CH₂ (a) → H₂ + (CH₃)₂CH (b)						
Hydrogen atom + Propane						
79 BAL/WAL1 k _a . A and B recalculated from an empirical formula proposed by the authors.	CO	753-773	1.32(14)	0	4715	2
76 SHE/KAL k _a + k _b .	EX	1123	3.7(12)			2
77 LED/VIL k _a + k _b .	EX	295	1.46(8)			2
78 LED/VIL k _a + k _b . Discharge-flow.	EX	281-1485	6.31(13)	0	3926±50	2 2.0
71 BAK/BAL k _b . Rate constant per secondary CH bond.	CO	298-753	5.1(13)	0	4253	2
79 BAL/WAL1 k _b . A and B recalculated from an empirical formula proposed by the authors.	CO	753-773	9.8(13)	0	4005	2
82 SHE/GUS k _b /k _a . Recalculated from the given secondary per primary bond rate constant ratio of 1.4±0.2. Pyrolysis of Propane/Isobutane mixtures, in a quartz flow-reactor. P = 100 torr.	RL	1023-1123	(4.7±0.7)(-1)			2/2
H + CH₂=CHCHO → products						
Hydrogen atom + 2-Propenal (Acrolein)						
78 KOD/NAK Fast flow-reactor. Time-of-flight Mass-spectrometry. P(Ar + H ₂) = 0.29 torr.	EX	298	(8.1±0.8)(11)			2
H + (CH₃)₂CO → H₂ + CH₃C(O)CH₂						
Hydrogen atom + 2-Propanone						
72 AZA/GYU	EX	843-928	(2.29±0.90)(14)	0	6995±755	2
76 AMB/BRA Discharge-flow. ESR detection.	EX	298-465	1.86(14)	0	3200±144	2 1.58

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
H + CH ₂ =CC=CH → CH=CCH=CH [†] (a) → CH=CC=CH ₂ [†] (b)						
Hydrogen atom + 1,3-Butadiyne						
75 SCH/WAR k _a + k _b .	EX	298	1.3(12)			2
H + CH ₂ =CCH=CH → products						
Hydrogen atom + 1-Buten-3-yne						
75 SCH/WAR	ES	298	(2.0±0.2)(12)			2
H + CH ₂ =CHCH=CH ₂ (+ M) → CH ₃ CHCH=CH ₂ (+ M) (a) → CH ₂ CH ₂ CH=CH ₂ (+ M) (b) → H ₂ + CH ₂ =CHCH=CH (+ M) (c) → H ₂ + CH ₂ =CCH=CH ₂ (+ M) (d)						
Hydrogen atom + 1,3-Butadiene						
71 DAB/NIK k _a + k _b . P(He) = 1.3 torr.	EX	298	(5.02±0.65)(12)			2
78 GOR/IVA2 ¹⁾	EX	305	(3.19±0.42)(11)			2
78 GOR/IVA2 ¹⁾ Lower-limit k.	EX	305	≥4.57(18)			3
¹⁾ k _a + k _b . Method based on collision-induced shifts and HF-transition line broadening in H atoms.						
79 ISH/SUG2 k _a + k _b . Pulse-radiolysis. Absorption-spectroscopy. P = (500-600) torr. H + (0.02-0.09) torr. OI.	EX	298	(5.12±0.90)(12)			2
79 OKA/CVE ²⁾ (k _a + k _b)/k _{ref} . k _{ref} : H + NO + M → HNO + M.	RL	298	(2.76±0.05)(-1)			2/3
79 OKA/CVE ²⁾ k _a + k _b .	RN	298	(4.27±0.26)(12)			2
²⁾ Modulated Hg-photosensitization. Chemiluminescence. k might be slightly P-dependent. The products are vibrationally excited. P = 100 torr.						
75 NAM/SHE k _a + k _b + k _c + k _d .	EX	1073-1123	(1.6±0.3)(13)	0	0	2
D + CH ₂ =CHCH=CH ₂ → CH ₂ DCBCH=CH ₂ (a) → CH ₂ CHDCBCH=CH ₂ (b)						
Deuterium atom + 1,3-Butadiene						
71 DAB/NIK k _a + k _b . M = He. P = (1.6-2.6) torr.	EX	298	(3.17±0.05)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 ISH/SUG2 $k_a + k_b$. Pulse-radiolysis. Absorption-spectroscopy. P = (500-600) torr. H_2 + (0.02-0.09) torr. OI.	EX	298	(4.52±0.36)(12)			2
H + CH ₃ CH ₂ CH=CH ₂ → CH ₃ CH ₂ CHCH ₃ (a) → CH ₃ CH ₂ CH ₂ CH ₂ (b) → H ₂ + CH ₃ CH ₂ CH=CH (c) → H + CH ₃ CH ₂ C=CH ₂ H (d) → H ₂ + CH ₃ CHCH=CH ₂ (e) (or H ₂ + CH ₃ CH=CHCH ₂) → H ₂ + CH ₂ CH ₂ CH=CH ₂ (f)						
Hydrogen atom + 1-Butene						
71 COW/KEI $k_a + k_b$. M = He. Discharge-flow. The products are vibrationally excited. P = 2.86 torr.	EX	298	(6.81±0.48)(11)			2
71 COW/KEI ¹⁾ ($k_a + k_b$)/ k_{ref} . k_{ref} : H + CH=CH → CH ₂ =CH [†]	RL	298	(2.96±0.58)(1)			2/2
71 COW/KEI ¹⁾ $k_a + k_b$.	RN	298	(7.83±2.41)(11)			2
¹⁾ M = Na, Ar. Steady-state Photolysis. The products are vibrationally excited. P = (10-15) torr.						
71 DAB/NIK $k_a + k_b$. M = Ha. P = (0.4-2.8) torr.	EX	298	(8.31±0.48)(11)			2
74 SHI/AMA ($k_a + k_b$)/($k_c + k_d + k_e + k_f$).	RL	923	1.5(1)			2/2
78 ISH/YAM $k_a + k_b$. Pulse-radiolysis. Resonance-absorption. Predominant paths. P(H_2) = (200-1200) torr.	EX	298	(1.20±0.30)(12)			2
79 OKA/CVE ²⁾ ($k_a + k_b$)/ k_{ref} . k_{ref} : H + NO + M → HNO + M.	RL	298	(4.94±0.13)(-2)			2/3
79 OKA/CVE ²⁾ $k_a + k_b$.	RN	298	(8.36±0.16)(11)			2
²⁾ Hg-photosensitization. Chemiluminescence. The products are vibrationally excited. P = 50 torr.						
82 HAR/FIT $k_a + k_b$. Flash-photolysis. Resonance-fluorescence. H atoms generated by pulsed vacuum-UV Photolysis of CH ₄ . P(Total) = 50 torr.	EX	298-445	(2.27±0.24)(13)	0	942±94	2
74 SHI/AMA k_a/k_b .	RL	923	3.0			2/2
72 FAL/SUN $k_e/(k_a + k_b)$.	RL	298	1.6(-2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$D + CH_3CH_2CH=CH_2 \rightarrow CH_3CH_2CHDCH_2$ (a) $\rightarrow CH_3CH_2CHCH_2D$ (b)						
Deuterium atom + 1-Butene						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.6-2.6) torr.	EX	298	(8.25±0.60)(11)			2
79 ISH/SAT $k_a + k_b$. Pulse-radiolysis. Resonance-absorption.	EX	298	(9.64±0.60)(11)			2
$H + CH_3CH=CHCH_3 \rightarrow CH_3CHCH_2CH_3$ (a) $\rightarrow H_2 + CH_3CH=CHCH_2$ (b) $\rightarrow H_2 + CH_3CH=CCH_3$ (c)						
Hydrogen atom + 2-Butene (Unspecified form)						
74 SHI/AMA $k_a/(k_b + k_c)$.	RL	923	5.0			2/2
74 LAU/BUE k_a/k_{ref} . k_{ref} : $H + CH_2=CH_2 \rightarrow CH_3CH_2^\dagger$ The product is vibrationally excited.	RL	298	(8.3±0.13)(-1)			2/2
$H + cis-CH_3CH=CHCH_3 \rightarrow H_2 + CH_3CH=CHCH_2$ (a) $\rightarrow H_2 + CH_3CHCH=CH_2$ (b) $\rightarrow CH_3CH_2CH(\cdot)CH_3$ (c)						
Hydrogen atom + 2-Butene, (Z)-						
72 FAL/SUN $(k_a + k_b)/k_c$.	RL	298	1.5(-2)			2/2
71 COW/KEI k_c . M = He. P = 3.24 torr. Discharge-flow. The product is vibrationally excited.	EX	298	(3.85±0.30)(11)			2
71 COW/KEI ¹⁾ k_c/k_{ref} . k_{ref} : $H + CH=CH \rightarrow CH_2=CH^\dagger$	RL	298	(9.1±0.9)			2/2
71 COW/KEI ¹⁾ k_c .	RN	298	(2.47±0.60)(11)			2
¹⁾ M = He. P = (10-15) torr. Steady-state Photolysis. The product is vibrationally excited.						
71 DAB/NIK k_c . M = He. P = (1.1-2.8) torr.	EX	298	(4.75±0.35)(11)			2
78 ISH/YAM k_c . Pulse-radiolysis. Resonance-absorption. The product is vibrationally excited. Predominant path. P(H ₂) = (200-1200) torr.	EX	298	(6.02±0.60)(11)			2
79 OKA/CVE ²⁾ k_{ref} : $H + NO + M \rightarrow HNO + M$.	RL	298	(2.29±0.05)(-2)			2/3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 OKA/CVE ²⁾ ²⁾ k _c . Hg-photosensitization. Chemiluminescence. The product is vibrationally excited. P = 50 torr.	RN	298	(3.62±0.06)(11)			2
82 HAR/PIT k _c . Flash-photolysis. Resonance-fluorescence. H atoms generated by pulsed vacuum-UV Photolysis of CH ₄ . Gas-chromatography. P(Total) = 50 torr.	EX	298-445	(1.74±0.18)(13)	0	1083±86	2
D + cis-CH₃CH=CHCH₃ → CH₃CHDCHCH₃						
Deuterium atom + 2-Butene, (Z)-						
71 DAB/NIK M = He. P = (0.6-2.6) torr.	EX	298	(4.07±0.22)(11)			2
79 ISH/SAT Pulse-radiolysis. Resonance-absorption.	EX	298	(4.82±0.60)(11)			2
H + trans-CH₃CH=CHCH₃ → H₂ + CH₃CH=CHCH₂ (a) → H₂ + CH₃CHCH=CH₂ (b) → CH₃CH₂CHCH₃ (c)						
Hydrogen atom + 2-Butene, (E)-						
72 FAL/SUN (k _a + k _b)/k _c .	RL	298	9.0(-3)			2/2
71 COW/KEI k _c . M = He. Discharge-flow. The product is vibrationally excited. P = 1.79 torr.	EX	298	(4.28±0.24)(11)			2
71 COW/KEI ¹⁾ k _c /k _{ref} . k _{ref} : H + CH=CH → CH ₂ =CH [†]	RL	298	(1.19±0.14)(1)			2/2
71 COW/KEI ¹⁾ k _c .	RN	298	(3.25±0.84)(11)			2
¹⁾ M = Ne, Ar. P = (10-15) torr. Steady-state Photolysis. The product is vibrationally excited.						
71 DAB/NIK k _c . M = He. P = (0.4-1.9) torr.	EX	298	(5.38±0.41)(11)			2
78 ISH/YAM k _c . Pulse-radiolysis. Resonance-absorption. Predominant path. P(H ₂) = (200-1200) T	EX	298	(6.63±1.20)(11)			2
78 KOD/NAK k _c . Fast-flow. P(Ar + H ₂) = 0.20 torr.	EX	298	(5.1±0.5)(11)			2
79 OKA/CVE ²⁾ k _{ref} : H + NO + M → HNO + M.	RL	298	(2.65±0.05)(-2)			2/3
79 OKA/CVE ²⁾ ²⁾ k _c . Hg-photosensitization. Chemiluminescence. The product is vibrationally excited. P = 50 torr.	RN	298	(4.55±0.08)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 HAR/PIT k_c . Resonance-fluorescence. H atoms generated by photolysis of CH_4 . P(Total) = 50 torr.	EX	298-445	(2.08±0.21)(13)	0	1043±63	2	
D + trans- $\text{CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CHDCHCH}_3$							
Deuterium atom + 2-Butene, (E)-							
71 DAB/NIK M = He. P = (0.7-2.2) torr.	EX	298	(4.66±0.14)(11)			2	
79 ISH/SAT Pulse-radiolysis. Resonance-absorption. Predominant path.	EX	298	(4.82±0.60)(11)			2	
H + $(\text{CH}_3)_2\text{C}=\text{CH}_2$ (+ M) \rightarrow $(\text{CH}_3)_3\text{C}$ (+ M) (a)							
$\rightarrow (\text{CH}_3)_2\text{CHCH}_2$ (+ M) (b)							
$\rightarrow \text{H}_2 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (+ M) (c)							
$\rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$ (+ M) (d)							
Hydrogen atom + 1-Propene, 2-methyl-							
76 BRA/WES1 k_a . Computer-fit to a proposed mechanism.	DE	1030-1300	1.6(13)	0	758	2	1.95
81 CAN/MAR1 k_a . Discharge-flow system. Mass-Spectrometry. P(Total) = (7-8) torr.	EX	298-563	3.89(13)	0	901±96	2	1.29
78 GOR/IVA2 $k_a + k_b$. Collision-induced shifts and HF-transition line broadening in H-atoms.	EX	305	(2.18±0.04)(12)			2	
78 GOR/IVA2 $k_a + k_b$. H-maser relaxation method.	EX	305	(2.17±0.60)(12)			2	
78 GOR/IVA2 $k_a + k_b$. Collision-induced shifts. HF-transition line broadening in H-atoms. Lower-limit k.	EX	305	≥3.08(18)			3	
78 HOR/CAL $(k_a + k_b)/k_{\text{ref}}$. HCHO Photolysis at 313 nm. P(HCHO) = (1-12) torr. k_{ref} : $\text{H} + \text{HCHO} \rightarrow \text{H}_2 + \text{CHO}$.	RL	298	(4.3±0.4)(1)			2/2	
78 ISH/YAM $k_a + k_b$. Pulse-radiolysis. Resonance-absorption. Predominant paths. P(H_2) = (200-1200) torr.	EX	298	(3.13±0.36)(12)			2	
79 OKA/CVE ¹⁾ $(k_a + k_b)/k_{\text{ref}}$. k_{ref} : $\text{H} + \text{NO} + \text{M} \rightarrow \text{HNO} + \text{M}$.	RL	298	(1.56±0.04)(-1)			2/3	
79 OKA/CVE ¹⁾ $k_a + k_b$.	RN	298	(2.43±0.09)(12)			2	
¹⁾ Hg-photosensitization. Chemiluminescence. The products vibrationally excited. P = 50 torr.							


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 HAR/PIT $k_a + k_b$. Flash-photolysis. Resonance-fluorescence. Gas-chromatography. H atoms generated by photolysis of CH_4 . P(Total) = 50 torr.	EX	298-445	(3.68±0.36)(13)	0	849±98	2
71 COW/KEI ²⁾ $(k_a + k_d)/k_{\text{ref}}$. k_{ref} : $\text{H} + \text{CH}=\text{CH} \rightarrow \text{CH}_2=\text{CH}^\dagger$	RL	298	(7.45±1.49)(1)			2/2 1.48
71 COW/KEI ²⁾ $k_a + k_d$.	RL	298	(2.05±0.60)(12)			2
²⁾ M = Ne, Ar. P = (10-15) torr. Steady-state Photolysis. Products vibrationally excited.						
76 BRA/WES2 k_b/k_a . Computer-fit to a proposed mechanism.	RL	1055-1325	6.76(-2)	0	-2382	2/2 1.48
78 MAR/PUR k_b/k_c . 2,2,3,3-Tetramethylbutane pyrolysis in a static system. P = (3-19) torr. Rate-ratio determined on the basis of reaction: $(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_3\text{C}$	RL	718	9.4(-1)			2/2
71 LEX/MAR2 k_d/k_a . M = Ar. Discharge flow. P(Ar) = (4-12) torr.	RL	290	(1.4±0.3)(-3)			2/2
80 MAR/CAN k_d/k_a . M = Ar. Discharge-flow. Products of (a) vibrationally excited. P(Ar) = 6.6 torr.	RL	293-601	2.95	0	1997±313	2/2
D + $(\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CDCH}_2$ (a) $\rightarrow (\text{CH}_3)_2\text{CCH}_2\text{D}$ (b)						
Deuterium + 1-Propene, 2-methyl-						
71 DAB/NIK M = He. P = (1.0-2.2) torr.	EX	298	(2.02±0.09)(12)			2
79 ISH/SAT $k_a + k_b$. Pulse-radiolysis. Resonance-absorption.	EX	298	(2.29±0.18)(12)			2
H + $(\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_3\text{CH}$ (a) $\rightarrow \text{H}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$ (b)						
Hydrogen atom + Ethyl, 1,1-dimethyl-						
71 LEX/MAR2 k_b/k_a . M = Ar. Discharge flow. Product of step (a) vibrationally excited. P(Ar) = (4-12) torr.	RL	290	(3.73±0.12)			2/2
80 MAR/CAN k_b/k_a . M = Ar. Discharge-flow. P(Ar) = 6.6 torr. T-independent ratio.	RL	293-601	(3.55±0.24)	0	0	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H} + (\text{CH}_3)_3\text{C}^\ddagger \rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CH} \quad (\text{a})$ $\rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 \quad (\text{b})$						
Hydrogen atom + Ethyl, 1,1-dimethyl-						
71 LEX/MAR2 ¹⁾	RL	290	(4.58±1.0)			2/2
k_a/k_{ref} .						
71 LEX/MAR2 ¹⁾	RL	290	(7.68±0.54)(-1)			2/2
k_b/k_{ref} .						
¹⁾ M = Ar. Discharge flow. P(Ar) = (4-12) torr.						
$k_{\text{ref}}: (\text{CH}_3)_3\text{C}^\ddagger + \text{M} \rightarrow (\text{CH}_3)_3\text{C} + \text{M}$						
$\text{H} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \quad (\text{a})$ $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CHCH}_3 \quad (\text{b})$						
Hydrogen atom + Butane						
79 BAL/WAL1	CO	753-773	1.32(14)	0	4715	2
k_a . A and B recalculated by an empirical formula.						
76 YAM/NAM	EX	980-1050	(9.64±2.53)(11)	0	0	2
$k_a + k_b$.						
71 BAK/BAL	CO	298-753	5.5(13)	0	4253	2
k_b . Rate constant per secondary CH bond.						
79 BAL/WAL1	CO	753-773	1.96(14)	0	4005	2
k_b . A and B recalculated by an empirical formula.						
$\text{H} + (\text{CH}_3)_3\text{CH} \rightarrow \text{H}_2 + (\text{CH}_3)_3\text{C} \quad (\text{a})$ $\rightarrow \text{H}_2 + (\text{CH}_3)_2\text{CHCH}_2 \quad (\text{b})$						
Hydrogen atom + Propane, 2-methyl-						
71 BAK/BAL	CO	298-753	8.7(13)	0	3553	2
k_a . Rate constant per tertiary CH bond.						
79 BAL/WAL1 ¹⁾	CO	753-773	5.1(13)	0	3030	2
k_a .						
79 BAL/WAL1 ¹⁾	CO	753-773	1.99(14)	0	4715	2
k_b .						
¹⁾ A and B recalculated by an empirical formula.						
82 SHE/GUS ²⁾	RL	1023-1123	(2.2±0.2)	0	0	2/2
$(k_a + k_b)/k_{\text{ref}}$.						
$k_{\text{ref}}: \text{H} + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{H}_2 + (\text{CH}_3)_2\text{CH} \quad (\text{c})$						
$\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 \quad (\text{d})$						
82 SHE/GUS ²⁾	RL	1023-1123	1.17	0	0	2/2
k_a/k_b . Recalculated from the reported tertiary per primary bond rate constant ratio of 10.5						
²⁾ Pyrolysis of Propane/Isobutane mixtures, in a quartz flow-reactor. P = 100 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 SHE/IVA $k_a + k_b$. Pyrolysis of $(\text{CH}_3)_3\text{CH}$ in various flow-reactors. P = (100-750) torr.	EX	1023-1073	$(8.0 \pm 0.9)(12)$	0	0	2
H + $(\text{CH}_3)_3\text{COH} \rightarrow \text{H}_2\text{O} + (\text{CH}_3)_3\text{C}$ Hydrogen atom + 2-Propanol, 2-methyl-						
73 ADE	EX	520-770	4.0(13)	0	4126	2
73 ADE/WAG2	EX	295-700	$(4.0 \pm 0.4)(13)$	0	4127 ± 302	2
H + $(\text{CH}_3\text{CH}_2)_2\text{O} \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{OCHCH}_3$ Hydrogen atom + Ethane, 1,1'-oxybis- (Diethyl ether)						
79 FAU/HOY Isothermal discharge-flow. Mass-spectrometry. Electron-Spin-Resonance. Gas-chromatography.	EX	250-620	$(7.4 \pm 3.6)(12)$	0	1630 ± 100	2
H +  $\rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{SH}$ Hydrogen atom + Thiophene, tetrahydro-						
78 HOR/NIS Discharge-flow technique. P ~ 5 torr.	DE	295-576	8.5(12)	0	1010	2
H + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SH} \rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{S}$ (a) $\rightarrow \text{H}_2\text{S} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ (b) Hydrogen atom + 1-Butanethiol						
78 HOR/NIS ¹⁾ k_a .	DE	295-576	1.3(13)	0	1600	2
78 HOR/NIS ¹⁾ k_b .	DE	295-576	1.6(12)	0	1119	2
¹⁾ Discharge-flow technique. P ~ 5 torr.						
H + $(\text{CH}_3\text{CH}_2)_2\text{S} \rightarrow \text{CH}_3\text{CH}_2\text{SH} + \text{CH}_3\text{CH}_2$ Hydrogen atom + Ethane, 1,1'-thiobis-						
81 EKW/SAF2 H atoms generated by Hg-photosensitized decomposition of H_2 . General-vacuum apparatus. Gas-chromatography. k determined relative to the reaction: $\text{H} + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2$. P(H_2) ~ 580 torr. P(Diethylsulfide) = (1-32) torr.	RN	298-461	$(4.7 \pm 0.9)(13)$	0	1911 ± 77	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
H + CH₃CH₂SSCH₂CH₃ → CH₃CH₂SH + CH₃CH₂S							
Hydrogen atom + Disulfide, diethyl-							
81 EKW/SAF1 H atoms generated by Hg-photosensitized decomposition of H ₂ . General-vacuum apparatus. Gas-chromatography. P(Diethyldisulfide) = (2-15) torr. P(H ₂) ~ 580 torr.	EX	298-418	(4.73±0.64)(13)	0	861±35	2	
H + CH₃CH₂CH₂CH=CH₂ → CH₃CH₂CH₂CHCH₃ (a)							
→ CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (b)							
→ H ₂ + CH ₃ CH ₂ CHCH=CH ₂ (c)							
→ H ₂ + CH ₃ CHCH ₂ CH=CH ₂ (d)							
→ H ₂ + CH ₂ CH ₂ CH ₂ CH=CH ₂ (e)							
Hydrogen atom + 1-Pentene							
71 COW/KEI k _a + k _b . M = He. Discharge-flow. The products are vibrationally excited. P = 3 torr.	EX	298	(6.38±0.48)(11)			2	
71 COW/KEI ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : H + CH=CH → CH ₂ =CH [†]	RL	298	(2.86±0.48)(1)			2/2	
71 COW/KEI ¹⁾ k _a + k _b . ¹⁾ M = Ne, Ar. Steady-state Photolysis. The products are vibrationally excited. P = (10-15) torr.	RN	298	(7.78±2.41)(11)			2	
74 SHI/AMA (k _a + k _b)/(k _c + k _d + k _e).	RL	923	9.0			2/2	
74 SHI/AMA k _a /k _b .	RL	923	3.0			2/2	
H + CH₃CH₂CH=CHCH₃ → CH₃CH₂CHCH₂CH₃ (a)							
→ CH ₃ CH ₂ CHCH ₂ CH ₃ (a)							
→ CH ₃ CH ₂ CH ₂ CHCH ₃ (b)							
→ H ₂ + CH ₃ CH ₂ CH=CHCH ₂ (c)							
→ H ₂ + CH ₃ CHCH=CHCH ₃ (d)							
→ H ₂ + CH ₂ CH ₂ CH=CHCH ₃ (e)							
Hydrogen atom + 2-Pentene (Unspecified form)							
74 SHI/AMA k _a /k _b .	RL	923	1.0			2/2	
74 SHI/AMA (k _a + k _b)/(k _c + k _d + k _e).	RL	923	3.0			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{H} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2$ (b) $\rightarrow \text{H}_2 + \text{CH}_3\text{CHC}(\text{CH}_3)=\text{CH}_2$ (c) $\rightarrow \text{H}_2 + \text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (d) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}_2\text{C}(=\text{CH}_2)\text{CH}_2$ (e)						
Hydrogen atom + 1-Butene, 2-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.7-1.3) torr.	EX	298	(9.09±0.96)(11)			2
74 SHI/AMA k_a/k_b .	RL	923	4.0			2/2
74 SHI/AMA $(k_a + k_b)/(k_c + k_d + k_e)$.	RL	923	1.3(1)			2/2
$\text{D} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)\text{CH}_2\text{D}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CD}(\text{CH}_3)\text{CH}_2$ (b)						
Deuterium atom + 1-Butene, 2-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (1.2-2.6) torr.	EX	298	(2.05±0.10)(12)			2
$\text{H} + (\text{CH}_3)_2\text{CHCHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCHCH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$ (b)						
Hydrogen atom + 1-Butene, 3-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.6-2.7) torr.	EX	298	(7.35±0.60)(11)			2
$\text{D} + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CHCHCH}_2\text{D}$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCHDCH}_2$ (b)						
Deuterium atom + 1-Butene, 3-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.6-2.6) torr.	EX	298	(7.65±0.60)(11)			2
$\text{H} + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_3\text{CHCH}(\text{CH}_3)_2$ (b) $\rightarrow \text{H}_2 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2$ (c) $\rightarrow \text{H}_2 + \text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2$ (d)						
Hydrogen atom + 2-Butene, 2-methyl- (Trimethylethylene)						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.7-1.3) torr.	EX	298	(8.19±1.02)(11)			2
74 LAU/BUE $(k_a + k_b)/k_{\text{ref}}$. $k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{H} \rightarrow \text{CH}_3\text{CH}_2^\ddagger$ The products are vibrationally excited.	RL	298	(1.25±0.29)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 SHI/AMA k_a/k_b .	RL	923	4.0			2/2
74 SHI/AMA $(k_a + k_b)/(k_c + k_d)$.	RL	923	3.0			2/2
78 ISH/YAM $k_a + k_b$. Pulse-radiolysis. Resonance-absorption.	EX	298	(1.45±0.18)(12)			2
D + CH₃CH=C(CH₃)₂ → CH₃CHCD(CH₃)₂ (a) → CH₃CHDC(CH₃)₂ (b)						
Deuterium atom + 2-Butene, 2-methyl-						
71 DAB/NIK $k_a + k_b$. M = He. P = (0.6-2.6) torr.	EX	298	(9.22±0.54)(11)			2
79 ISH/SAT $k_a + k_b$. Pulse-radiolysis. Resonance-absorption.	EX	298	(1.20±0.18)(12)			2
H + CH₃CH₂CH₂CH₂CH₃ → H₂ + CH₃CH₂CH₂CH₂CH₂ (a) → H₂ + CH₃CH₂CH₂CHCH₃ (b) → H₂ + CH₃CH₂CHCH₂CH₃ (c)						
Hydrogen atom + Pentane						
79 BAL/WAL1 ¹⁾ k_a .	CO	753-773	1.32(14)	0	4715	2
79 BAL/WAL1 ¹⁾ $k_b + k_c$.	CO	753-773	2.94(14)	0	4005	2
¹⁾ A and B recalculated by an empirical formula.						
H + (CH₃)₂CHCH₂CH₃ → H₂ + CH₂CH(CH₃)CH₂CH₃ (a) → H₂ + (CH₃)₂CHCH₂CH₂ (b) → H₂ + (CH₃)₂CHCHCH₃ (c) → H₂ + (CH₃)₂CCH₂CH₃ (d)						
Hydrogen atom + Butane, 2-methyl-						
79 BAL/WAL1 ¹⁾ $k_a + k_b$.	CO	753-773	1.98(14)	0	4715	2
79 BAL/WAL1 ¹⁾ k_c .	CO	753-773	9.8(13)	0	4005	2
79 BAL/WAL1 ¹⁾ k_d .	CO	753-773	5.1(13)	0	3030	2
¹⁾ A and B recalculated by an empirical formula.						
H + (CH₃)₄C → H₂ + (CH₃)₃CCH₂						
Hydrogen atom + Propane, 2,2-dimethyl- (Neopentane)						
76 BAK/BAL k_{ref} : O ₂ + H → O + OH. Optimization.	RL	753	5.2(1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 BAK/BAL	ES	753	2.4(11)			2	
79 BAL/WAL1	CO	753-773	2.64(14)	0	4715	2	
A and B recalculated by an empirical formula.							
H + (CH₃)₃COCH₃ → products							
Hydrogen atom + Propane, 2-methoxy-2-methyl-							
79 FAU/HOY	EX	250-620	(1.4±0.8)(14)	0	3750±150	2	
Isothermal discharge-flow.							
Electron-Spin-Resonance.							
Gas-chromatography.							
Mass-spectrometry.							
H + CH₃CH₂CH₂C(CH₃)=CH₂ → CH₃CH₂CH₂C(CH₃)₂ (a)							
→ CH ₃ CH ₂ CH ₂ CH(CH ₃)CH ₂ (b)							
→ H ₂ + CH ₃ CH ₂ CHC(CH ₃)=CH ₂ (c)							
→ H ₂ + CH ₂ CH ₂ CH ₂ C(CH ₃)=CH ₂ (d)							
→ H ₂ + CH ₃ CH ₂ CH ₂ C(=CH ₂)CH ₂ (e)							
Hydrogen atom + 1-Pentene, 2-methyl-							
74 SHI/AMA	RL	923	4.0			2/2	
k _a /k _b .							
74 SHI/AMA	RL	923	8.0			2/2	
(k _a + k _b)/(k _c + k _d + k _e).							
H + CH₃CH₂CH=C(CH₃)₂ → CH₃CH₂CH₂C(CH₃)₂ (a)							
→ CH ₃ CH ₂ CHCH(CH ₃) ₂ (b)							
→ H ₂ + CH ₃ CH ₂ CH=C(CH ₃)CH ₂ (c)							
→ H ₂ + CH ₃ CHCH=C(CH ₃) ₂ (d)							
Hydrogen atom + 2-Pentene, 2-methyl-							
74 SHI/AMA	RL	923	3.0			2/2	
k _a /k _b .							
74 SHI/AMA	RL	923	3.0			2/2	
(k _a + k _b)/(k _c + k _d).							
H + CH₃CH₂C(CH₃)=CHCH₃ → CH₃CH₂C(CH₃)CH₂CH₃ (a)							
→ CH ₃ CH ₂ CH(CH ₃)CHCH ₃ (b)							
→ H ₂ + CH ₃ CH ₂ C(CH ₃)=CHCH ₂ (c)							
→ H ₂ + CH ₃ CHC(CH ₃)=CHCH ₃ (d)							
→ H ₂ + CH ₃ CH ₂ C(=CH ₂ CH ₃)CH ₂ (e)							
Hydrogen atom + 2-Pentene, 3-methyl-							
74 SHI/AMA	RL	923	3.0			2/2	
k _a /k _b .							
74 SHI/AMA	RL	923	3.0			2/2	
(k _a + k _b)/(k _c + k _d + k _e).							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$H + (CH_3)_2C=C(CH_3)_2 \rightarrow (CH_3)_2CCH(CH_3)_2$ Hydrogen atom + 2-Butene, 2,3-dimethyl- (Tetramethylethylene)						
71 DAB/NIK M = He. P = (0.7-1.3) torr.	EX	298	(6.99±0.30)(1)			2
$D + (CH_3)_2C=C(CH_3)_2 \rightarrow (CH_3)_2CCD(CH_3)_2$ Deuterium atom + 2-Butene, 2,3-dimethyl- (Tetramethylethylene)						
71 DAB/NIK M = He. P = (0.6-2.6) torr.	EX	298	(8.55±0.78)(11)			2
$D + \text{Cyclohexane} \rightarrow DH + \text{Cyclohexyl}^\bullet$ Deuterium atom + Cyclohexane → Deuterium hydride + Cyclohexyl						
75 KIM/TIM Reaction of D atom with Cyclohexane in an ESR-flow. Mass-spectrometry. [Cyclohexane] = (0.48-1.32)10 ¹⁴ molec.cm ⁻³ . P = (0.33-0.94) torr.	EX	297-596	(4.1±1.0)(13)	0	2013±151	2
$H + CH_3(CH_2)_4CH_3 \rightarrow H_2 + CH_3(CH_2)_4CH_2$ (a) $\rightarrow H_2 + CH_3CH_2CH_2CH_2CHCH_3$ (b) $\rightarrow H_2 + CH_3CH_2CH_2CHCH_2CH_3$ (c) $\rightarrow H_2 + CH_3CH_2CHCH_2CH_2CH_3$ (d)						
Hydrogen atom + Hexane						
81 SHE/RUM ¹⁾	EX	973	(8.8±2.7)(12)			2
81 SHE/RUM ¹⁾	EX	1028	(8.7±2.2)(12)			2
¹⁾ k _a + k _b + k _c + k _d . Flow-reactor with powdered-quartz-fluidized bed. P(Hexane) = (10-50) torr. P(Total) = 100 torr.						
$H + (CH_3)_2CHCH(CH_3)_2 \rightarrow H_2 + (CH_3)_2CHCH(CH_3)CH_2$ (a) $\rightarrow H_2 + (CH_3)_2CCH(CH_3)_2$ (b)						
Hydrogen atom + Butane, 2,2-dimethyl-						
75 BUL/MAR k _b /k _a . Estimated ratio. Static System pyrolysis.	RL	667-770	1.0(-1)	0	-2526	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$H + (CH_3)_2CHN=NCH(CH_3)_2$ $\rightarrow H_2 + CH_2CH(CH_3)N=NCH(CH_3)_2$ (a) $\rightarrow (CH_3)_2CHNHNCH(CH_3)_2$ (b)						
Hydrogen atom + Diazene, bis(1-methylethyl)- (Azoisopropane)						
72 ARI/STE k_a/k_b . Azoisopropane Photolysis.	RL	295	(1.0±0.15)(-1)			2/2
$H + (CH_3)_3CCH(CH_3)_2 \rightarrow H_2 + (CH_3)_3CC(CH_3)_2$ (a) $\rightarrow H_2 + CH_2(CH_3)_2CCH(CH_3)_2$ (b) $\rightarrow H_2 + (CH_3)_3CCH(CH_3)CH_2$ (c)						
Hydrogen atom + Butane, 2,2,3-trimethyl-						
81 BAL/WAL2 ¹⁾ k_a/k_{ref} . $k_{ref}: H + O_2 \rightarrow OH + O$. Estimated ratio.	RL	753	1.64(2)			2/2
81 BAL/WAL2 ¹⁾ $(k_b + k_c)/k_{ref}$. $k_{ref}: H + O_2 \rightarrow OH + O$. Estimated ratio.	RL	753	9.3(1)			2/2
81 BAL/WAL2 ¹⁾ $(k_a + k_b + k_c)/k_{ref}$. $k_{ref}: H + O_2 \rightarrow OH + O$. Optimization.	RL	753	2.57(2)			2/2
81 BAL/WAL2 ¹⁾ $k_a + k_b + k_c$.	SE	753	1.48(12)			2
¹⁾ Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric acid- coated reaction vessels. Gas-chromatography. P(2,2,3-Trimethylbutane) = 5 torr. P(Total) = 500 torr.						
$H + (CH_3)_3CC(CH_3)_3 \rightarrow H_2 + (CH_3)_3CC[(CH_3)_2]CH_2$						
Hydrogen atom + Butane, 2,2,3,3-tetramethyl						
78 MAR/PUR 2,2,3,3-Tetramethylbutane pyrolysis in a static system. P = (3-19) torr. k_{ref} : $H + (CH_3)_2C=CH_2 \rightarrow H_2 + CH_2C(CH_3)=CH_2$ Rate ratio determined on the basis of reaction: $(CH_3)_3CC(CH_3)_3 \rightarrow (CH_3)_3C + (CH_3)_3C$	RL	699-735	1.0(1)	0	2045±3609	2/2 100.



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
H₂ (+ M) → H + H (+ M)							
Hydrogen molecule							
73 BRE/BIR M = H.	EX	3500-8000	2.12(15)	0	43885	2	
73 BRE/BIR M = H ₂ .	EX	3500-8000	3.30(15)	0	52944	2	
73 BRE/BIR M = Ar.	EX	3500-8000	9.35(13)	0	44741	2	
73 BRE/BIR M = Xe.	EX	3500-8000	9.35(13)	0	44741	2	
D₂ (+ M) → D + D (+ M)							
Deuterium molecule							
75 APF/APF	EX	1800-4000	1.45(14)	0	47006	2	
H₂ + D₂ → HD + HD							
Hydrogen molecule + Deuterium molecule							
77 LIF/FRE	ES	1200-1516	1.26(14)	0	19124±2516	2	6.31
HD + HD → H₂ + D₂							
Deuterium hydride							
72 NIK/MAI Pressure-normalized rate constant.	EX	833-1022	1.26(22)	0	28083±1808	2	15.85
H₂ + NO → H + HNO							
Hydrogen molecule + Nitrogen oxide (NO)							
75 KOS/AND	EX	2000-4000	3.98(13)	0	29039	2	
76 AND/ASA Reevaluation of the experimental data reported in 75 KOS/AND by using a computer simulation method.	DE	2300-3500	3.16(13)	0	27781	2	1.41

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
H₂(v>5) + NO → H + HNO						
Hydrogen molecule + Nitrogen oxide (NO)						
80 DOD/ZEL High-frequency discharge. Mass-spectrometry.	EX	295	(1.20±0.60)(13)			2
H₂ + NO₂ → H + HONO						
Hydrogen molecule + Nitrogen oxide (NO ₂)						
78 SLA/GRI2 Shock-waves. Fit to experimental data. P = (1-4) atm.	ES	760-1000	(2.4±1.0)(13)	0	14595±503	2
H₂ + N₂O → H₂O + N₂						
Hydrogen molecule + Nitrogen oxide (N ₂ O)						
78 ROO/HAN Shock-waves. Estimated k on the basis of a suggested mechanism. The preexponential factor expressed as: A(T/298) ^{0.5} .	ES	1700-3000	3.45(12)	0.5	0	2
H₂(X¹Σ_g⁺) + C₂(X¹Σ_g⁺) → H(2S) + CH≡C(X²Σ⁺) (a) → CH=CH (b)						
Hydrogen molecule + Carbon dimer						
79 PAS/MCD k _a . Multiphoton laser photodissociation of CF ₃ C≡CCF ₃ . Laser-induced fluorescence.	EX	298	(8.31±0.36)(11)			2
82 PIT/PAS k _b . Dye-laser induced fluorescence. Carbon dimers produced by multiphoton UV-photolysis of CF ₃ C≡CCF ₃ .	EX	300-600	(1.07±0.66)(14)	0	1470±216	2
80 REI/MAN2 k _{overall} . IR Multiple photon dissociation CH ₂ =CHCN or CHCl=CCl ₂ . Laser-induced Fluorescence.	EX	300	(8.43±1.20)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err. factor
$H_2(X^1\Sigma_g^+) + C_2(a^3\Pi_u) \rightarrow H(^2S) + CH\equiv C(X^2\Sigma^+)$ (a)							
\rightarrow any other products (b)							
Hydrogen molecule + Carbon dimer							
81 PAS/PIT	EX	300-600	(9.34±0.60)(12)	0	3012±31	2	
k_a . Multiple photon laser dissociation of $CF_3C\equiv CCF_3$ or C_6H_6 . Laser-Induced Fluorescence.							
80 REI/MAN2	EX	300	<1.81(10)			2	
$k_a + k_b$. IR Multiple photon dissociation of $CH_2=CHCN$ or $CHCl=CCl_2$. Laser-induced Fluorescence. Upper-limit k.							
$D_2 + C_2(a^3\Pi_u) \rightarrow D + CD\equiv C$							
Deuterium molecule + Carbon dimer							
81 PAS/PIT	EX	300-600	(1.08±0.13)(13)	0	3710±72	2	
Multiple photon laser dissociation of $CF_3C\equiv CCF_3$ or C_6H_6 . Laser-induced Fluorescence.							
$H_2 + C_2O \rightarrow$ products							
Hydrogen molecule + Carbon oxide (C_2O)							
80 DON/PIT	EX	298	<1.20(11)			2	
Laser photodissociation of C_3O_2 at 266 nm. Dye-laser Induced Fluorescence. Upper-limit k.							
$D_2 + CH\equiv CH \rightarrow CHD=CHD$							
Deuterium molecule + Ethyne							
77 OGU2	EX	1000-1600	(4.9±1.3)(11)	0	17564±302	2	
$H_2 + C_3 \rightarrow$ products							
Hydrogen molecule + Carbon trimer							
80 REI/MAN1	EX	300	≤1.80(10)			2	
IR Multiphoton dissociation of Allene. Time-Resolved Chemiluminescence. Upper-limit k.							
$H_2 +$ \rightarrow							
Hydrogen molecule + 1,3-Cyclohexadiene → Cyclohexene							
72 DEM/HUY	EX	512-673	1.78(13)	0	18319±554	2	2.51
Pyrolysis in a cylindrical Pyrex reaction vessel. Gas-chromatography. Mass-spectrometry. P = (10-500) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + O₃ → HO₂ + O₂						
Hydroxyl + Ozone						
73 AND/KAU2	EX	220-450	7.83(11)	0	956	2
73 DEM	EX	300	4.81(10)			2
73 KUR	EX	298	(3.91±0.60)(10)			2
74 SIM/HEI1	ES	298	≥9.03(9)			2
Lower-limit k.						
74 SIM/HEI1	ES	298	(3.01±1.81)(10)			2
75 DEM	RL	271-333	1.68(1)	0	1233	2/2
k _{ref} : CO + OH → CO ₂ + H.						
75 DEM	RN	271-333	1.51(12)	0	1233	2
Estimated k.						
78 CHA/KAU	ES	295	(3.76±0.15)(10)			2
Laser-induced fluorescence technique.						
79 RAV/WIN1	EX	238-357	(1.10±0.21)(12)	0	930±50	2
Flash-photolysis. Resonance-fluorescence.						
See RAV/WIN2 for erratum.						
80 ZAH/HOW	RN	300	(3.91±0.60)(9)			2
Discharge-flow. Laser Magnetic Resonance.						
OH(v=n) + O₃ → HO₂ + O₂ (a)						
→ OH + O + O ₂ (b)						
→ H + O ₂ + O ₂ (c)						
Hydroxyl + Ozone						
71 COL/WOR ¹⁾	EX	298	(1.14±0.66)(12)			2
v = 2.						
71 COL/WOR ¹⁾	EX	298	(4.64±0.18)(12)			2
v = 9.						
¹⁾ k _a + k _b + k _c .						
71 POT/COL	EX	298	(4.64±0.18)(12)			2
k _a + k _b + k _c . v = 9.						
76 STR/JOH ¹⁾	EX	300	(2.23±0.06)(12)			2
v = 4.						
76 STR/JOH ¹⁾	EX	300	(6.63±2.41)(12)			2
v = 9.						
¹⁾ k _a + k _b + k _c .						
OD(v=n) + O₃ → DO₂ + O₂ (a)						
→ OD + O + O ₂ (b)						
→ D + O ₂ + O ₂ (c)						
Hydroxyl-d + Ozone						
74 BAS/ORA	EX	298	(3.31±0.54)(12)			2
k _a + k _b + k _c .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + H₂ → H₂O + H							
Hydroxyl + Hydrogen molecule							
71 BRA/BEL1	EX	1100-1600	2.1(13)	0	2567±151	2	2.57
71 EBE/HOY	DE	500-1600	1.0(13)	0	2416	2	
72 DIX ¹)	RL	1050	(1.13±0.70)(1)			2/2	
k _{ref} : OH + CO → CO ₂ + H.							
72 DIX ¹)	RL	298-1330	(1.20±0.15)(2)	0	2400±50	2/2	
k _{ref} : OH + CO → CO ₂ + H.							
Combination of present and other data.							
72 DIX ¹)	ES	1050	(2.7±0.4)(12)			2	
72 DIX ¹)	SE	298-1330	3.72(13)	0	2770±100	2	
Combination of present and other data.							
¹) Fuel-rich H ₂ /N ₂ /O ₂ flames.							
72 STU/NIK1	EX	298	4.28(9)			2	1.15
73 DAY/THO	ES	1050	(2.7±0.4)(12)			2	
73 DAY/THO	RL	298-1330	(1.20±0.15)(2)	0	2400±50	2/2	
Estimated ratio.							
73 GAR/MAL	EX	1200-2500	5.2(13)	0	3271	2	1.20
73 SMI/ZEL2	EX	210-460	1.4(13)	0	2416	2	
73 WES/DEH1	EX	298-745	4.6(9)			2	
Non-linear Arrhenius behavior.							
Within the given T-range, k increases							
k increases from 4.6x10 ⁹ to							
4.0x10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ .							
74 GAR/MAL	EX	1350-1600	5.2(13)	0	3248	2	
74 GAR/MAL	SE	300-1800	7.57(11)	1.77	1528	2	
Combination of present and other data.							
The preexponential factor expressed							
as: A(T/298) ^{1.77} .							
74 SMI/ZEL	EX	298	(4.28±0.06)(9)			2	
74 SMI/ZEL	EX	210-460	(1.08±0.54)(13)	0	2334±120	2	
75 ATK/HAN1	EX	298	(4.20±0.42)(9)			2	
75 ATK/HAN2	EX	297-434	3.55(12)	0	2008±151	2	
75 ATK/HAN2	EX	298	(4.20±0.42)(9)			2	
75 OVE/PAR	EX	295	(3.49±0.16)(9)			2	
75 TRA/ROS	EX	300	3.91(9)			2	
H ₂ O is vibrationally excited.							
75 VAN/PEE	EX	600-1300	7.0(12)	0	2214	2	
76 BRA/CAP	RL	1300	5.9(-1)			2	
k _{ref} : OH + CH ₄ → H ₂ O + CH ₃							
77 SHA	ES	250-2000	1.33(12)	0.75	1575	2	
The preexponential factor expressed							
as: A(T/298) ^{0.75} .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 BIE/ZET2 M = He. Pulsed vacuum UV-Photolysis. Resonance-absorption. P(He) = 740 torr.	EX	297	(4.3±0.5)(9)			2	
78 PRE Laser Magnetic Resonance Spectrometry.	EX	293	(2.6±0.7)(9)			2	
79 COH/WES Critical review. The preexponential factor expressed as: $A(T/298)^{1.3}$. $\Delta \log k = 0.1$ at 300 K, 0.15 for the (250-500) K range, and 0.3 at 2000 K.	RE	250-3000	1.81(12)	1.3	1835	2	
79 ZEL Critical evaluation. Best fit of all available experimental data. The preexponential factor expressed as: $A(T/298)^{1.6}$.	SE	300-2000	9.09(11)	1.6	1660	2	
80 SWO/HOC Flash-photolysis of H ₂ O vapor. P ~ 760 torr.	EX	296	(5.1±1.1)(9)			2	
80 TUL/RAV M = Ar. Flash-photolysis. Resonance-fluorescence. Non-linear, best-fit Arrhenius expression. The preexponential factor expressed as: $A(T/298)^{2.44}$. P(H ₂) = (0-1) torr. P(H ₂ O) = 150 torr. P(Ar) = 50 torr.	EX	298-992	2.70(11)	2.44	1281	2	
81 RAV/NIC M = Ar. Flash-photolysis of H ₂ /H ₂ O/Ar mixtures. Resonance-fluorescence. Low-T, linear Arrhenius expression. P(Ar) ~ 100 torr.	EX	250-400	(2.95±0.30)(12)	0	1990±340	2	
OH(v=1) + H₂ → H₂O + H							
Hydroxyl + Hydrogen molecule							
77 SPE/END Upper-limit k.	EX	295	<6.02(9)			2	
OH(v=n) + H₂(v=1) → H₂O + H							
Hydroxyl + Hydrogen molecule							
78 LIG/MAT n = 0. Flow-tube with tunable dye laser. Upper-limit k.	EX	298	≤3.3(12)			2	
81 GLA/CHA n = 0. Discharge-flow system. OH produced by reacting H with NO ₂ . EPR-spectroscopy. P(H ₂) = (1-2) torr.	EX	296	(6.0±1.5)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 ZEL/STE n = 0. H ₂ (v=1) generated in a flow system by passing H ₂ over a heated W filament. OH enerated by reacting H with NO ₂ . Resonance-fluorescence. [H ₂ (v=1)] = (0.562.70)x10 ¹⁴ molec.cm ³ . [OH] ₀ = 4.9x10 ¹² molec.cm ⁻³ . [H ₂] ~ 5.010 ¹⁶ molec.cm ⁻³ .	EX	298	(4.5±1.8)(11)			2	
78 LIG/MAT n = 1. Flow-tube with tunable dye laser. Upper-limit k.	EX	298	≤5.7(12)			2	
OH + HD → HDO + H							
Hydroxyl + Deuterium hydride							
72 DIX ¹⁾	RL	1050	(2.8±0.42)			2/2	
k _{ref} : OH + HD → HOD + H.							
72 DIX ¹⁾	RL	1050	2.4	0	-155	2/2	
k _{ref} : OH + HD → HOD + H. Estimated ratio.							
72 DIX ¹⁾	ES	1050	(9.6±0.5)(11)			2	
¹⁾ Fuel-rich H ₂ /N ₂ /O ₂ flames.							
73 DAY/THO	ES	1050	(9.6±0.5)(11)			2	
OH + D₂ → HDO + D							
Hydroxyl + Deuterium molecule							
72 STU/NIK1	EX	298	1.153(9)			2	1.15
74 SMI/ZEL	EX	298	(1.33±0.24)(9)			2	
74 SMI/ZEL	EX	210-460	(7.53±0.36)(12)	0	2586±180	2	
80 PAR/NIP	EX	297	(1.27±0.11)(9)			2	
Flash-photolysis. Resonance-absorption.							
81 RAV/NIC ¹⁾	EX	250-1050	2.19(12)	1.18	2332	2	
M = Ar. Non-linear Arrhenius expression over the whole T-range. The preexponential factor expressed as: A(T/298) ^{1.18} .							
81 RAV/NIC ¹⁾	EX	250-470	(7.29±3.13)(12)	0	2670±150	2	
M = Ar. n = 0 assumed. Low T-range.							
¹⁾ Flash-photolysis of D ₂ /H ₂ O/Ar mixtures. Resonance-fluorescence. P(Ar) ~100 torr.							
OH + H₂ → HDO + H							
Hydroxyl-d + Hydrogen molecule							
80 PAR/NIP	EX	297	(3.70±0.25)(9)			2	
Flash-photolysis. Resonance-absorption.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A units	k err. factor
OD + D₂ → D₂O + D							
Hydroxyl-d + Deuterium molecule							
75 APP/APP Data-fit.	ES	1700-3100	6.63(13)	0	2592	2	3.02
80 PAR/NIP Flash-photolysis. Resonance-absorption.	EX	297	(1.33±0.13)(9)			2	
OH + OH (+ M) → H₂O + O (+ M) (a) → HO ₂ + H (+ M) (b) → H ₂ O ₂ (+ M) (c)							
Hydroxyl							
73 GAR/MAL 1)	EX	1200-2500	5.5(13)	0	3523	2	1.25
73 MCK/MUL 1)	EX	298	(1.3±0.3)(12)			2	
73 WES/DEH2 1) 1) k _a .	EX	298	(1.4±0.2)(12)			2	
74 CLY/DOW 2)	EX	300	(1.02±0.36)(12)			2	
74 CLY/DOW 2) k based on present and previous data.	SE	300	(8.43±1.20)(11)			2	
2) k _a . Discharge-flow. Resonance-fluorescence.							
74 RAW/GAR2 3) n = 0 assumed.	RN	1200-2000	5.5(13)	0	3488	2	
74 RAW/GAR2 3) Data fit. B = 0 assumed. The preexponential factor expressed as: A(T/298) ^{1.11} .	CO	1200-2000	1.19(12)	1.11	0	2	
74 RAW/GAR2 3) Data fit. The preexponential factor expressed as: A(T/298) ^{2.03} .	CO	1200-2000	1.77(11)	2.03	-600	2	
3) k _a .							
74 TRA/ROS1 k _a . H ₂ O is vibrationally excited.	EX	298	(1.26±0.12)(12)			2	
77 ERN/WAG 4)	EX	1180-1820	3.4(13)	0	2526	2	
77 ERN/WAG 4) Modified Arrhenius expression based on weighed absolute values of all available data.	SE	300-2000	9.92(11)	1.14	0	2	
77 ERN/WAG 4) Modified Arrhenius expression. Transition-State Theory calculation. E _a = 0 at 300 K and ~2400 calmol ⁻¹ in the (1000-2000) K range.	CO	300-2000	7.29(11)	1.23	0	2	
4) k _a . Shock heating of HONO ₂ /Ar mixtures. The preexponential factor expressed as: A(T/298) ⁿ in the modified Arrhenius expressions.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 SHA k _a . The preexponential factor expressed as: $A(T/298)^{0.75}$.	ES	250-2000	1.33(12)	0.75	0	2	
79 ZEL k _a . 5) $k = \exp(27.1 + 1.5 \times 10^{-3}T) \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ Critical evaluation. Non-Arrhenius best-fit of all available experimental data.	SE	300-2000	5)	5)	5)	2	
80 FAR/SMI k _a . Discharge flow. Resonance-fluorescence.	EX	298	(1.02±0.12)(12)			2	
81 WAG/ZEL k _a . Alternative non-Arrhenius expression over the extended T-range (250-2000) K: $k = 6.02 \times 10^{23} \exp(-27.73 + 1.49 \times 10^{-3}T) \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. Flash-photolysis of H ₂ O/N ₂ mixtures. UV-Resonance spectrometry. P < 100 torr.	EX	250-580	(1.93±0.48)(12)	0	242	2	
79 HAC/PRE1 k _b . Isothermal flow-reactor. Laser Magnetic Resonance. $k_1 = k_{-1}K$. P(Total) = (130-800) Pa.	DE	298	1.1(-16)			2	
74 TRA/ROS1 k _c . M = N ₂ .	EX	298	(9.07±1.09)(16)			3	
OH + HO₂ → H₂O + O₂							
Hydroxyl + Hydroperoxo							
72 DAY/DIX k _{ref} : H + HO ₂ → H ₂ + O ₂ . Upper-limit ratio.	RL	300-1800	≤5.5			2/2	
72 FRI/SUT	ES	2130	1.2(13)			2	
72 HOC/GHO	EX	298	(1.2±0.2)(14)			2	
73 DAY/THO k _{ref} : H + HO ₂ → H ₂ + O ₂ . Upper-limit ratio.	RL	300-1050	≤5.5			2/2	
73 PEE/MAH1	ES	1600	≈5.0(13)			2	
74 DEM/TSC	ES	298	9.64(13)			2	3.0
75 GLA/TRO Upper-limit k.	EX	1350-1700	≤4.0(13)			2	
75 HAC/HOY Upper-limit k.	EX	298-670	≤2.0(13)			2	
77 BUR/HAR	EX	293	(3.07±0.96)(13)			2	
78 CHA/KAU Discharge-flow. Best fit between experiments and computer calculations.	DE	295	(1.5±0.3)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 COX Photolysis of Cl ₂ /H ₂ /NO ₂ in N ₂ /O ₂ . P = 1 atm.	ES	283	(9.03±0.30)(12)			2	
78 HAC/PRE Isothermal discharge-flow. P(He) = 1.9 torr.	EX	293	(1.8±0.6)(13)			2	
78 PRE Laser Magnetic Resonance Spectrometry.	EX	293	(1.8±0.6)(13)			2	
79 BUR/CLI Discharge-flow.	EX	298	(3.07±1.02)(13)			2	
79 DEM Photolysis of H ₂ /O ₂ /O ₃ (or N ₂) mixtures. Average of six reported k values.	RN	298	(9.8±2.4)(13)			2	
80 HOC/SWO2 H ₂ O flash-photolysis in presence of O ₂ and CO (or He). P = 760 torr.	EX	296	(7.0±1.5)(13)			2	
80 LII/GOR2 Electron pulse-radiolysis. Kinetic Spectrophotometry. P(Total) = 1200 torr.	EX	308	(5.96±0.72)(13)			2	
80 TEM/WAG Discharge-flow. Laser Magnetic Resonance.	EX	296	(3.9±1.5)(13)			2	
81 BUR/COX Photolysis O ₃ /H ₂ O/O ₂ mixtures in presence of N ₂ or He. Molecular Modulation. T-independent in the given T-range. P(Total) = 760 torr.	DE	288-348	(3.73±2.41)(13)	0	0	2	
81 COX/BUR Low-frequency square-wave modulated Photolysis of O ₃ /H ₂ O mixtures. P = 760 torr.	EX	308	(6.0±1.5)(13)			2	
81 KEY Discharge-flow Resonance-fluorescence. Mass-spectrometry. P(Total) = 1 torr.	EX	299	(3.9±0.9)(13)			2	
81 SRI/QIU HO ₂ produced by reacting F with H ₂ O ₂ . Discharge-flow. Laser-induced Fluorescence. Resonance-fluorescence. P ~3 torr. [H ₂ O ₂] ~ (6-26) × 10 ¹² molec. cm ⁻³ . [HO ₂] ~ (2-19) × 10 ¹¹ molec. cm ⁻³ . [OH] ₀ = (4-6) × 10 ¹⁰ molec. cm ⁻³ . [H ₂ O] ~ 5 × 10 ¹³ molec. cm ⁻³ . [F ₂] ~ 6 × 10 ¹³ molec. cm ⁻³ .	EX	296	(4.5±0.7)(13)			2	
81 THR/WIL1 Laser magnetic resonance spectrometry.	EX	298	(3.5±0.5)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 BRA/HOF H ₂ O flash-photolysis in N ₂ , with or without O ₂ . P(H ₂ O) = (0.2-2.1) torr. P(Total) = 750 torr. P(N ₂) = (728-984) torr. P(O ₂) = (0-17) torr.	ES	298	6.6(13)			2	1.3
82 DEM H ₂ O photolysis with O ₂ in traces. Laser-induced fluorescence. P(Total) = (75-730) torr. He, or Ar.	EX	298	(7.2±2.4)(13)			2	
82 TEM/WAG1 Reaction of OH with HO ₂ in several isothermal discharge-flow-reactors. OH generated by reacting F with H ₂ O. HO ₂ generated by reacting OH with H ₂ O ₂ . [OH] ₀ = (1.93-3.79)x10 ¹² molec.cm ⁻³ . [H ₂ O ₂] = (0.36-4.82)x10 ¹³ molec.cm ⁻³ . P = (1.5-10.5) torr. k is independent within this P-range.	EX	296	(4.0±1.4)(13)			2	
OH(v=9) + H₂O → products							
Hydroxyl + Water							
72 WOR/COL Lower-limit k. Unreported T assumed to be 298 K.	EX	298	≥1.20(11)			2	
OH + H₂O₂ → HO₂ + H₂O							
Hydroxyl + Hydrogen peroxide							
72 GOR/VOL	EX	298	(7.23±0.18)(11)			2	
72 VOL/GOR	EX	298	(7.23±0.18)(11)			2	
73 GOR	RN	298	(7.47±0.48)(11)			2	
74 HAC/HOY2	EX	298-669	(4.8±1.0)(12)	0	670±70	2	
75 HAC/HOY	EX	298-670	(4.8±1.0)(12)	0	670±70	2	
75 MEA/HEI k _{ref} : OH + CO → H + CO ₂	RL	298	(4.1±0.6)			2/2	
78 PRE Laser Magnetic Resonance Spectrometry.	EX	293	(4.8±1.0)(11)			2	
79 HAR/PIT Flash-photolysis. Resonance-fluorescence.	EX	298	(4.1±0.8)(11)			2	
80 KEY Discharge-flow. Resonance-fluorescence. P(Total) = (1-4) torr.	EX	245-423	(1.5±0.4)(12)	0	126±76	2	
80 SRI/REI Discharge-flow. Laser-induced fluorescence. [H ₂ O ₂] = (0.6-5.0)x10 ¹³ molec.cm ⁻³ . P(He) = (2-3) torr.	EX	250-459	(1.8±0.3)(12)	0	164±52	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 TEM/WAG Discharge-flow. Laser Magnetic Resonance.	EX	296	(1.05±0.20)(12)			2
81 NEL/MAR M = Ar. Flash-photolysis combined with: either Resonance-fluorescence [P(Total) = 10-50 torr.], or Laser absorption [P(Total) = 10 torr.]	EX	295	(9.46±0.60)(11)			2
81 WIN/SEM ¹⁾	EX	273-410	(2.23±0.36)(12)	0	260±50	2
81 WIN/SEM ¹⁾ Average k of 80 KEY, 80 SRI/REI and 81 WIN/SEM data.	SE	273-410	(1.70±0.18)(12)	0	167±35	2
1) Flash-photolysis of H ₂ O ₂ in He, or SF ₆ . Resonance-fluorescence. P(Total) = 100 torr. He, or 40 torr. SF ₆ . [H ₂ O ₂] = (0.36-3.60)×10 ¹⁵ molec.cm ⁻³ .						
82 KUR/MJR Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H ₂ O ₂ /Ar mix- tures. [H ₂ O] ~ 100 mtorr. [Ar] = (20-30) torr. [H ₂ O ₂] = (0-20) mtorr.	EX	250-370	(1.75±0.18)(12)	0	161±32	2
82 MAR/JOH Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H ₂ O ₂ . P(Ar) = 10 torr.	EX	298	(1.9±0.14)(12)			2
82 MOL/MOL Flash-photolysis. Resonance-fluorescence. UV-, and IR-spectrophotometry. P = 760 torr.	EX	294	(1.08±0.18)(12)			2
82 TEM/WAG1 Reaction of OH with H ₂ O ₂ in several isothermal discharge-flow reactors. OH generated by reacting F with H ₂ O. P = (1.5-10.5) torr. k is P-independent within this P-range. [OH] ₀ = (0.57-2.59)×10 ¹¹ molec.cm ⁻³ . [H ₂ O ₂] = (0.36-6.02)×10 ¹³ molec.cm ⁻³ .	EX	296	(1.0±0.2)(12)			2
OH + S → H + SO						
Hydroxyl + Sulfur atom						
79 JOU/LEB2 Discharge-flow reactor. EPR-spectrometer.	EX	298	(3.98±0.84)(13)			2
OH + SO → H + SO₂						
Hydroxyl + Sulfur monoxide						
79 JOU/LEB2 Discharge-flow reactor. EPR-spectrometer.	EX	298	(5.06±0.90)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + SO₂ (+ M) → HOSO₂ (+ M)						
Hydroxyl + Sulfur dioxide						
74 COX2 Expressed as k[M], with M = N ₂ + O ₂ at 1 atm.	RN	294	(3.61±0.48)(11)			2
75 CAS/DAV Pseudo-second order k. M = N ₂ . Limiting high-pressure k. P = 760 torr.	EX	298	3.6(11)			2
75 COX Expressed as k[M], with M = N ₂ + O ₂ at 1 atm.	RN	300	(3.61±0.48)(11)			2
75 GOR/MUL1 M = He. In an atmosphere of Water vapor.	EX	435	(1.08±0.05)(12)			2
76 ATK/PER3 M = Ar. P = 760 torr.	EX	298	(4.04±0.42)(11)			2
76 ATK/PER3 M = Ar. Limiting high-pressure k.	ES	298	≈5.00(11)			2
77 CAS/TAN M = N ₂ . Limiting high-pressure k. P = 760 torr.	EX	297	3.61(11)			2
77 CAS/TAN The product is vibrationally excited.	EX	297	4.28(11)			2
79 DAV/RAV M = N ₂ . Flash-photolysis. Resonance-fluorescence. P = 760 torr. High-pressure k.	EX	298	5.42(11)			2
80 COX/SHE ¹) k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(9.0±2.0)(-2)			2/2
80 COX/SHE ¹) ¹) Photolysis of HONO and SO ₂ . Gas-chromatography. P = 760 torr.	RN	297	(4.34±0.96)(11)			2
80 HAR/ATK ²) M = Ar.	EX	298-424	6.99(9)	0	-1193±151	2
80 HAR/ATK ²) M = Ar.	EX	298	(3.91±0.51)(11)			2
80 HAR/ATK ²) M = SF ₆ .	EX	298-424	7.65(10)	0	-752±151	2
80 HAR/ATK ²) M = SF ₆ .	EX	298	(9.70±1.33)(11)			2
80 HAR/ATK ²) M = N ₂ .	ES	298-424	2.41(10)	0	-956	2
80 HAR/ATK ²) M = N ₂ .	ES	298	6.02(11)			2
²) Flash-photolysis. Resonance-fluorescence. P(Total) ~ 650 torr. High-pressure k's.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 PAY/STI M = N ₂ (18 torr.) + H ₂ O(20 torr.)	RN	300	5.44(16)			3	
75 CAS/DAV M = N ₂ . Low-pressure k. P < 20 torr.	EX	298	5.80(16)			3	
75 HAR/WAY M = N ₂ . M-efficiencies relative to N ₂ are: 1.0(N ₂), 0.63(Ar).	EX	298	(2.61±0.94)(17)			3	
76 ATK/PER3 M = Ar. Limiting low-pressure k.	EX	298	(5.95±1.20)(16)			3	
77 CAS/TAN M = N ₂ . Low-pressure k.	EX	297	5.80(16)			3	
77 CAS/TAN Low-pressure k. Expression based on the experimental values k(297) and E _a . n = 0 assumed.	EX	253-297	5.05(14)	0	-1409	3	
77 CAS/TAN Low-pressure k. The preexponential factor expressed as: A(T/298) ^{-5.1} .	EX	253-297	6.11(16)	-5.1	0	3	
82 LEU ³) M = He. n = 0 assumed.	EX	261-414	(1.31±0.36)(15)	0	-913±74	3	
82 LEU ³) M = He. P = (0.9-10.0) torr.	EX	261-414	(2.87±0.09)(16)	-2.85	0	3	
82 LEU ³) M = Ar. P = (1.0-3.6) torr.	EX	298	(3.95±0.33)(16)			3	
82 LEU ³) M = N ₂ . P = (0.9-4.0) torr.	EX	298	(9.21±1.20)(16)			3	
82 LEU ³) M = O ₂ . P = (1.7-2.3) torr.	EX	298	(8.92±1.16)(16)			3	
82 LEU ³) M = CO ₂ . P = (0.6-1.7) torr.	EX	298	(4.35±1.12)(17)			3	
82 LEU ³) M = SO ₂ . n = 0 assumed.	EX	261-414	(1.93±0.98)(16)	0	-908±129	3	
82 LEU ³) M = SO ₂ . P = (0.02-0.20) torr.	EX	261-414	(4.17±0.33)(17)	-2.78	0	3	
³) Discharge-flow. Resonance-fluorescence. OH generated by reacting H with NO ₂ . Low-pressure k's. The preexponential factors expressed as: A(T/298) ⁿ . [OH] ₀ = (1.0-5.0)x10 ¹¹ molec.cm ⁻³ .							
OH(v=9) + SO ₂ → HOSO ₂ Hydroxyl + Sulfur dioxide							
72 WOR/COL Lower-limit k. Unreported T assumed to be 298 K.	EX	298	≥1.45(10)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + H₂S → H₂O + SH						
Hydroxyl + Hydrogen sulfide						
72 NIK/MOR1	ES	300	~5.12(12)			2
73 WES/DEH3	EX	298-885	1.4(13)	0	443	2
73 WES/DEH3	EX	298	(3.3±0.2)(12)			2
74 STU2	EX	298	(1.87±0.30)(12)			2
76 PER/ATK1	EX	297-427	(3.13±0.30)(12)	0	0	2
76 PER/ATK1	EX	298	(3.16±0.32)(12)			2
80 COX/SHE ¹⁾	RL	297	(6.2±0.4)(-1)			2/2
k _{ref} : OH + CH ₂ =CH ₂ → products.						
80 COX/SHE ¹⁾	RN	297	(3.01±0.18)(12)			2
¹⁾ HONO/H ₂ S photolysis. P = 760 torr.						
81 WIN/KRE	EX	244-367	(3.85±0.78)(12)	0	55±58	2
Flash-photolysis of H ₂ O/Ar/H ₂ S mixtures. Resonance-fluorescence. P(Ar) = (40-120) torr. P(H ₂ O) = (0.05-0.19) torr.						
82 LEU/SMI1 ²⁾	EX	228-518	(3.55±0.36)(12)	0	89	2
n = 0 assumed.						
82 LEU/SMI1 ²⁾	EX	228-518	(2.16±0.15)(11)	2.5	-725	2
The preexponential factor expressed as: A(T/298) ^{2.5} .						
²⁾ Discharge-flow. Resonance-fluorescence. Mass-spectrometry. OH generated by reacting H with NO ₂ . [OH] ₀ = (0.6-4.0) × 10 ¹¹ molec. cm ⁻³ .						
82 LIN	EX	239-425	(4.70±1.57)(12)	0	146±105	2
Flash-photolysis. Resonance-fluorescence. OH generated by UV-photolysis of H ₂ O near 308 nm.						
82 MIC/NAV ³⁾	EX	228	(3.08±0.23)(12)			2
82 MIC/NAV ³⁾	EX	298	(2.66±0.22)(12)			2
82 MIC/NAV ³⁾	EX	437	(3.35±0.29)(12)			2
82 MIC/NAV ³⁾	EX	228-437	(3.01±0.33)(12)	0	0	2
Average value.						
³⁾ Reaction of H ₂ S with OH in Ar. Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of H ₂ O. P(Ar) = (20-120) torr. P(H ₂ S) = (0.8-8.0) mtorr. P(H ₂ O) = (32-238) mtorr.						
OH(v=9) + H₂S → products						
Hydroxyl + Hydrogen sulfide						
72 WOR/COL	EX	298	≥1.51(11)			2
Lower limit k. Unreported T assumed to be 298 K.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + N₂ → H + N₂O						
Hydroxyl + Nitrogen molecule						
75 ALB/HOY k obtained from k ₋₁ and thermodynamic data.	DE	700-1100	3.2(12)	0	40512	2
OH(v=9) + N₂ → products						
Hydroxyl + Nitrogen molecule						
72 WOR/COL	EX	298	(2.17±0.30)(9)			2
OH + NO (+ M) → HONO (+ M)						
Hydroxyl + Nitrogen oxide (NO)						
72 STU/NIK2 M = He. Limiting high-pressure k.	EX	300	(1.20±0.60)(12)			2
74 COX2 M = N ₂ + O ₂ . P = 1 atm. k expressed as k[M].	RN	294	(3.67±0.66)(12)			2
75 ATK/HAN1 M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.85(Ar). P = 760 torr.	EX	298	(3.67±0.60)(12)			2
75 ATK/HAN1 Extrapolated limiting high-pressure k.	ES	298	4.81(12)			2
75 COX M = N ₂ + O ₂ . P = 1 atm. k expressed as k[M].	RN	300	(3.67±0.78)(12)			2
75 GOR/MUL1 M = H ₂ O. In an atmosphere of water vapor.	EX	435	(4.5±0.2)(12)			2
76 BLA/OVE M = H ₂ O. M-efficiencies relative to H ₂ O are: 1.00(H ₂ O), 0.02(He), 0.12(N ₂), 0.37(SF ₆), 0.41(CF ₄). Flash-photolysis. Resonance-absorption. Limiting high-pressure k.	EX	295	(1.1±0.1)(13)			2
76 COX/DER1 k _{ref} : OH + H ₂ → H ₂ O + H. M = N ₂ + O ₂ . P = 1 atm.	RL	298	(1.63±0.24)(3)			2/2
76 COX/DER1 M = N ₂ + O ₂ .	RN	298	(7.05±1.02)(12)			2
76 OVE/PAR M = H ₂ O, CF ₄ , SF ₆ , N ₂ , Ar, or He. Limiting high-pressure k. The product is vibrationally excited.	EX	295	(1.11±0.10)(12)			2
76 SIE/SIM2 M = 80% H ₂ , (18-20)% N ₂ O, (1-2)% CO. k _{ref} : OH + CO → H + CO ₂ . P = (408-768) torr.	RL	298	(2.2±0.3)(1)			2/2
76 SIE/SIM2 M = 63% H ₂ , 30% N ₂ O, 7% CO. P = 96 torr. k _{ref} : OH + CO → H + CO ₂ .	RL	298	(1.61±0.2)(1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 SIE/SIM2 Limiting high-pressure k.	RN	298	7.23(12)			2
76 SIM/HEI $k_{ref}: OH + H_2 \rightarrow H_2O + H.$	RL	296	(4.83±0.50)(2)			2/2
76 SIM/HEI M = H ₂ . P ~ 100 torr.	ES	296	2.23(12)			2
76 SIM/HEI M = H ₂ . P ~ 730 torr.	ES	296	6.63(12)			2
78 ANA/SMI1 ¹⁾	EX	233	7.83(12)			2
78 ANA/SMI1 ¹⁾	EX	296	4.04(12)			2
78 ANA/SMI1 ¹⁾	EX	298	5.12(12)			2
78 ANA/SMI1 ¹⁾	EX	405	6.63(12)			2
78 ANA/SMI1 ¹⁾	EX	505	4.22(12)			2
¹⁾ Flash-photolysis. Resonance-absorption. High-pressure k. P = 1 atm.						
79 CAM/PAR Boric-acid-coated Pyrex reaction vessels. P = 100 torr.	EX	292	(8.2±1.2)(11)			2
72 AND/KAU M = Ar. P = 5 torr.	EX	297	(1.45±0.73)(17)			3
72 AND/KAU M = Ar. P = 8 torr.	EX	297	(9.07±0.36)(16)			3
72 MOR/SMI M = He. Low-pressure k.	EX	300	(1.49±0.22)(12)			3
72 MOR/SMI M = He. Low-pressure k.	EX	416	6.89(16)			3
72 MOR/SMI M = He. Low-pressure k. Based on the given E _a and the experimental k's at 300 K and 416 K.	CO	300-416	1.00(16)	0	-806±241	3
72 WES/DEH4 M = He. k decreasing within the given T-range from 4.7x10 ¹⁷ to 1.3x10 ¹⁷ cm ⁶ mol ⁻¹ s ⁻¹ .	EX	273-395	4.7(17)			3
72 WES/DEH4 M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 2.23(He).	EX	298	1.3(17)			3
74 AND/MAR M = He.	EX	230-450	6.58(15)	0	-856±151	3 1.2
74 AND/MAR M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.57(He), 0.59(Ar). P(Ar) = (1-10) torr. P(He) = (1-10) torr. P(N ₂) = (2-5) torr.	EX	295	(2.10±0.44)(17)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 HOW/EVE M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.51(He), 0.56(Ar).	EX	296	2.83(17)			3	
75 ATK/HAN1 M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.70(Ar). Low-pressure k.	EX	298	(2.21±0.25)(17)			3	
75 HAR/WAY M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.47(Ar).	EX	298	(5.44±1.81)(17)			3	
78 ANA/SMI1 ²) M = N ₂ . Limiting low-pressure k.	EX	233	4.17(17)			3	
78 ANA/SMI1 ²) M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.37(He), 0.50(Ar). Limiting low-pressure k.	EX	296	2.97(17)			3	
78 ANA/SMI1 ²) M = N ₂ . Limiting low-pressure k.	EX	405	1.05(17)			3	
78 ANA/SMI1 ²) M = N ₂ . Limiting low-pressure k. ²) Flash-photolysis. Resonance-absorption.	EX	505	8.71(17)			3	
OH(v=9) + NO → HONO							
Hydroxyl + Nitrogen oxide (NO)							
72 WOR/COL	EX	298	(9.03±1.81)(10)			2	
OH + NO₂ (+ M) → HO₂ + NO (+ M) (a) → HONO₂ (+ M) (b)							
Hydroxyl + Nitrogen oxide (NO ₂)							
75 GLA/TRO k _a . Increasing to 1.9x10 ¹² cm ³ mol ⁻¹ s ⁻¹ at 1700 K.	ES	1350	≈7.0(11)			2	
80 HOW k _a . Discharge-flow. Laser Magnetic Resonance.	EX	452-1115	(1.82±0.36)(13)	0	3360±135	2	
72 SIM/HEI2 k _b . M = H ₂ O. Limiting high-pressure k.	RN	300-423	6.3(12)	0	171	2	
74 GLA/TRO1 k _b . M = Ar. Limiting high-pressure k. The preexponential factor expressed as: A(T/298) ^{-0.85} . k ₁ k ₋₁ K.	DE	295-1200	3.14(12)	-0.85	0	2	1.58
75 GOR/MUL1 k _b . M = H ₂ O. IN an atmosphere of water vapor.	EX	435	3.2(12)			2	
76 ANA/SMI k _b . M = N ₂ . Limiting high-pressure k.	EX	296	9.78(12)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 ATK/PER3 k _b . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.92(Ar). P = 760 torr.	EX	298	(3.85±0.60)(12)			2
76 ATK/PER3 k _b . M = Ar, or N ₂ . Limiting high-pressure k.	ES	298	≈5.12(12)			2
78 ANA/SMI3 ¹⁾	EX	220	1.20(13)			2
78 ANA/SMI3 ¹⁾	EX	296	9.64(12)			2
78 ANA/SMI3 ¹⁾	EX	358	7.83(12)			2
78 ANA/SMI3 ¹⁾	EX	450	2.29(12)			2
78 ANA/SMI3 ¹⁾	EX	550	2.65(12)			2
¹⁾ k _b . M = N ₂ . Flash-photolysis. Resonance- absorption. Limiting high-pressure k's.						
79 CAM/PAR ²⁾	EX	292	(2.5±0.4)(12)			2
k _b . M = CO. P = 100 torr.						
79 CAM/PAR ²⁾	EX	292	(1.2±0.3)(12)			2
k _b . M = N ₂ . P = 5.49 torr.						
²⁾ Boric-acid-coated Pyrex reaction vessels.						
79 O'B/GRE k _b . Photolysis of an Air/H ₂ O/NO _x mixture. P(Air) = 780 torr. P(H ₂ O) = 11 torr.	EX	301	(7.83±1.81)(12)			2
79 WIN/KRE ³⁾	EX	247	(1.10±0.09)(12)			2
[N ₂] = 5.4x10 ¹⁷ molec.cm ⁻³ . M-efficiencies relative to N ₂ are: 0.35(He), 0.55(Ar), 1.00(N ₂), 1.7(SF ₆).						
79 WIN/KRE ³⁾	EX	297	(6.00±0.46)(11)			2
[N ₂] = 5.4x10 ¹⁷ molec.cm ⁻³ . M-efficiencies relative to N ₂ are: 0.45(He), 0.65(Ar), 1.00(N ₂), 2.6(SF ₆).						
79 WIN/KRE ³⁾	EX	297	6.63(12)			2
P(N ₂) = 760 torr.						
79 WIN/KRE ³⁾	EX	352	(4.10±0.30)(11)			2
[N ₂] = 5.4x10 ¹⁷ molec.cm ⁻³ . M-efficiencies relative to N ₂ are: 0.45(He), 0.60(Ar), 1.00(N ₂), 2.9(SF ₆).						
³⁾ k _b . M = N ₂ . Flash-photolysis. Resonance-fluores- cence. k values reported for different [M] up to 2.3x10 ¹⁹ molec.cm ³ , in the T-range (247-352) K.						
80 AND k _b . Limiting high-pressure k. The preexponential factor expressed as: A(T/298) ^{-1.6} . Discharge-flow. Resonance-fluorescence.	CO	220-1100	7.23(12)	-1.6	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 ROB/SMI k_b . Pulsed-photolysis of HONO ₂ in Ar, or CF ₄ . High-pressure k. P(Ar) = 4 atm. P(CF ₄) = 8.6 atm. [N ₂] = 3.2x10 ¹⁷ -4.0x10 ¹⁸ molec.cm ⁻³ .	EX	295	≈1.81(13)			2	
72 AND/KAU k_b . M = Ar. M-efficiencies relative to Ar are: 1.0(Ar), 2.0(N ₂).. Low-pressure k. P(Ar) = 3 torr. P(N ₂) = 8 torr.	EX	297	(3.63±1.09)(17)			3	
72 SIM/HEI2 k_b . M = H ₂ O. Limiting low-pressure k.	RN	300-423	4.0(18)	0	0	3	
72 WES/DEH4 k_b . M = He. k decreasing within the given T-range from 7.3x10 ¹⁷ to 2.1x10 ¹⁷ cm ³ mol ⁻¹ s ⁻¹ .	EX	273-395	7.3(17)			3	
72 WES/DEH4 k_b . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 1.9(He).	EX	298	3.0(17)			3	
74 AND/MAR k_b . M = Ar.	EX	230-450	1.68(16)	0	-906±151	3	1.2
74 AND/MAR k_b . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.43(He), 0.43(Ar). P(He) = (1-10) torr. P(Ar) = (1-10) torr. P(N ₂) = (1-8) torr.	EX	295	(8.34±1.81)(17)			3	
74 GLA/TRO1 ⁴⁾ k_b . M = He. Limiting low-pressure, concentra- tion-dependent expression = k/[He]. $k_1 = k_{-1}K$.	DE	295-1200	5.84(17)	-2.98	0	3	1.58
74 GLA/TRO1 ⁴⁾ k_b . M = Ar. Limiting low-pressure, concentra- tion-dependent expression = k/[Ar]. $k_1 = k_{-1}K$.	DE	295-1200	3.75(17)	-2.9	0	3	1.58
⁴⁾ The preexponential factors expressed as: A(T/298) ⁿ .							
74 GLA/TRO1 k_b . M = N ₂ . Limiting low-pressure, concentra- tion-dependent expression = k/[N ₂]. $k_1 = k_{-1}K$.	DE	622	3.0(17)			3	
74 GLA/TRO1 k_b . M = N ₂ . Limiting low-pressure, concentra- tion-dependent Arrhenius expression = k/[N ₂]. Determined by using $k_1 = Kk_{-1}$.	DE	670	1.7(17)			3	
74 HOW/EVE k_b . M = N ₂ .	EX	296	1.05(18)			3	
75 HAR/WAY k_b . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.58(Ar).	EX	298	(9.43±3.63)(17)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 ANA/BEM k_b . M = N ₂ . Resonance absorption. Limiting low-pressure k. k decreases from $2.0 \times 10^{18} \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$ at T = 220K, to $5.9 \times 10^{17} \text{ cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$ at T = 358K. [N ₂] = 3.2×10^{17} - $4.0 \times 10^{18} \text{ molec. cm}^{-3}$.	EX	220	1.96(18)				3
76 ANA/SMI k_b . M = N ₂ . Limiting low-pressure k. M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.34(He), 0.42(Ar), 0.68(O ₂), 2.53(SF ₆).	EX	296	9.43(17)				3
76 ANA/SMI k_b . M = N ₂ . Limiting low-pressure k. n = 0 assumed. A and B recalculated from the reported data.	EX	220-550	(5.26±1.78)(16)	0	-818±79		3
76 ANA/SMI k_b . M = N ₂ . Limiting low-pressure k. The A-factor recalculated from the reported experimental data. The preexponential factor expressed as: $A(T/298)^{-2.6}$.	EX	220-550	(9.67±2.18)(17)	-2.6	0		3
76 ATK/PER3 k_b . M = Ar. Limiting low-pressure k.	EX	298	(3.70±0.36)(17)				3
77 ERL/FIE k_b . M = He. Low pressure k. The preexponential factor expressed as: $A(T/298)^{-2.9}$.	EX	213-300	(3.60±0.97)(17)	-2.9	0		3
77 ERL/FIE k_b . M = He. Low-pressure k. M-efficiencies relative to He are: 1.00(He), 4.00(CO ₂).	EX	300	(3.63±1.45)(17)				3
78 ANA/SMI ⁵⁾ k_b . M = N ₂ .	EX	220	2.29(18)				3
78 ANA/SMI ⁵⁾ k_b . M = N ₂ .	EX	296	9.61(17)				3
78 ANA/SMI ⁵⁾ k_b . M = N ₂ .	EX	358	6.06(17)				3
78 ANA/SMI ⁵⁾ k_b . M = N ₂ .	EX	450	3.95(17)				3
78 ANA/SMI ⁵⁾ k_b . M = N ₂ .	EX	550	2.21(17)				3
78 ANA/SMI ⁵⁾ k_b . M = He.	EX	220	9.07(17)				3
78 ANA/SMI ⁵⁾ k_b . M = He.	EX	296	3.30(17)				3

⁵⁾ Flash-photolysis. Resonance-absorption.
Limiting low-pressure k's.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err. factor
78 ANA/SMI3 ⁶⁾ k _b . M = He.	EX	220	1.09(18)			3	
78 ANA/SMI3 ⁶⁾ k _b . M = He.	EX	296	3.81(17)			3	
⁶⁾ Discharge-flow. Resonance-fluorescence. Limiting low-pressure k's.							
80 AND ⁷⁾ k _b . M = N ₂ . Limiting low-pressure k. P(N ₂) = (0.8-2.0) torr. n = 0 assumed.	EX	225-389	(5.80±1.45)(16)	0	-785±136	3	
80 AND ⁷⁾ k _b . The preexponential factor expressed as: A(T/298) ^{-2.9} . P(N ₂) = (0.8-2.0) torr.	EX	225-389	(8.34±2.18)(17)	-2.9	0	3	
80 AND ⁷⁾ k _b . M = He. Limiting low-pressure k. P(He) = (1.5-2.7) torr.	EX	298	(6.17±0.73)(17)			3	
⁷⁾ Discharge-flow. Resonance-fluorescence.							
OH + N₂O (+ M) → HO₂ + N₂ (+ M) (a) → products (b)							
Hydroxyl + Nitrogen oxide (N ₂ O)							
76 BIE/ZET k _a .	EX	298	(2.29±0.72)(7)			2	
77 CHA/KAU k _a . Upper-limit k.	EX	480	≤2.41(8)			2	
75 GOR/MUL1 k _b . M = H ₂ O. Upper-limit k. In an atmosphere of Water vapor.	EX	440	<1.0(10)			2	
76 ATK/PER2 k _b . M = Ar. Limiting high-pressure, upper-limit k.	EX	298-443	≤1.20(8)			2	
OH(v=9) + N₂O → products							
Hydroxyl + Nitrogen oxide (N ₂ O)							
72 WOR/COL	EX	298	(2.89±1.33)(10)			2	
OH + NH₂ → products							
Hydroxyl + Amidogen							
80 FEN Lean-burnt gas mixture. Average ratio. k _{ref} : NO + NH ₂ → N ₂ + H ₂ O.	RL	1110-1500	(1.0±0.5)(1)	0	0	2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + NH₃ → H₂O + NH₂							
Hydroxyl + Ammonia							
73 GEH/HOY	EX	298	1.7(11)			2	
73 KUR	EX	298	(2.47±0.36)(10)			2	
73 STU3	EX	298	(9.03±2.41)(10)			2	
74 DOV/NIP	EX	1620-1920	≤3.85(11)	0.68	554	2	
Upper-limit k. Preexponential factor expressed as: $A(T/298)^{0.68}$.							
74 HAC/HOY1	EX	298-669	(3.2±0.5)(12)	0	920	2	
74 HAC/HOY1	EX	298	(1.3±0.3)(13)			2	
74 ZEL/SMI	EX	230-490	1.39(12)	0	805	2	1.07
74 ZEL/SMI	EX	298	9.52(10)			2	
75 COX/DER2	ES	296	(7.23±2.41)(10)			2	
75 GOR/MUL1	EX	418	(2.6±0.3)(11)			2	
M = H ₂ O. In an atmosphere of Water vapor.							
75 SMI/ZEL	EX	228-472	1.39(12)	0	805	2	1.07
75 ZEL	EX	228-472	1.4(12)	0	800	2	
Flash-photolysis. Resonance-absorption.							
76 PER/ATK1	EX	297-427	1.76(12)	0	861±151	2	
76 PER/ATK1	EX	298	(9.88±0.96)(10)			2	
79 PAG/ERI ¹⁾	EX	300	(1.6±0.2)(11)			2	
79 PAG/ERI ¹⁾	EX	298-365	(6.89±0.86)(11)	0	438±40	2	
Based on the experimental k at 300 K and the reported E _a .							
¹⁾ Gaseous NH ₃ pulse-radiolysis.							
80 FEN	ES	1235	3.0(11)			2	
Lean-burnt gas mixture. Tentative k.							
80 SIL/KOL	EX	294-1075	(3.26±0.52)(12)	0	1067±72	2	
Discharge-flow. Mass-spectrometry.							
81 FUJ/MIY1 ²⁾	SE	300-2200	3.16(12)	0	1007	2	
Obtained by combining the present data with those reported in 74 HAC/HOY.							
81 FUJ/MIY2 ²⁾	EX	1360-1840	3.09(12)	0	981±75	2	1.1
²⁾ Oxidation of NH ₃ behind reflected shock-waves, in NH ₃ /H ₂ /O ₂ /Ar mixtures.							
81 NIE/WAG ³⁾	EX	300-1400	(2.5±1.0)(12)	0	980	2	
n = 0 assumed.							
81 NIE/WAG ³⁾	EX	300-1400	3.15(11)	1.05	350	2	
The preexponential factor expressed as: $A(T/298)^{1.05}$.							
³⁾ OH radicals generated by H ₂ O photolysis at 165-185 nm. Shock-waves. Flash-photolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + NH₂NH₂ → products							
Hydroxyl + Hydrazine							
74 HAC/HOY1	EX	298	1.3(13)			2	1.2
79 HAR/ATK ¹⁾	EX	298-424	2.65(13)	0	-116±176	2	
M = Ar. P(Ar) = (25-50) torr.							
79 HAR/ATK ¹⁾	EX	298-424	(3.67±0.60)(13)	0	0	2	
B = 0 assumed.							
¹⁾ Flash-photolysis. Resonance-fluorescence.							
OH + HNO → H₂O + NO							
Hydroxyl + Nitrosyl hydride							
72 SMI	EX	2100	(1.08±0.12)(13)			2	
75 CAM/HAN2	RL	425	≤4.4			2/2	
k _{ref} : O + HNO → H ₂ + NO. Upper-limit ratio.							
OH + HONO → H₂O + NO₂							
Hydroxyl + Nitrous acid							
74 COX1	RL	300	(3.7±0.6)(-1)			2/2	
k _{ref} : OH + NO + M. → HONO + M.							
74 COX1	RN	300	1.08(12)			2	
74 COX2	RN	294	(1.33±0.12)(12)			2	
75 COX	RN	300	(1.33±0.12)(12)			2	
75 COX/DER2	ES	296	2.17(12)			2	
76 COX/DER1	RL	298	(9.45±0.48)(2)			2/2	
k _{ref} : OH + H ₂ → H ₂ O + H.							
76 COX/DER1	RN	298	(3.98±0.18)(12)			2	
76 COX/DER2	RL	298	(9.04±0.94)(2)			2/2	
k _{ref} : OH + CH ₄ → H ₂ O + CH ₃ .							
76 COX/DER3	RL	296	(3.25±0.44)(-1)			2/2	
k _{ref} : OH + CH ₃ CHO → H ₂ O + CH ₃ CO							
76 FIF	RN	1000-1400	(1.55±0.5)(12)	0	0	2	
76 FIF	RN	1000-1400	6.92(12)	0	1761	2	
B = 0 assumed.							
OH + HONO₂ → H₂O + NO₃ (a)							
→ H ₂ O ₂ + NO ₂ (b)							
→ [HO.HONO ₂] [†] (c)							
Hydroxyl + Nitric acid							
72 MOR/SMI ¹⁾	EX	300	(7.82±3.01)(10)			2	
74 GLA/TRO1 ¹⁾	EX	1000-1100	(9.5±2.0)(10)	0	0	2	
74 ZEL/SMI ¹⁾	EX	240-405	(5.42±1.20)(10)	0	0	2	
75 MAR/KAU1 ¹⁾	EX	270-470	(5.36±0.78)(10)	0	0	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 SMI/ZEL ¹⁾ 1) k_a .	EX	240-406	(4.82±1.20)(10)	0	0	2	
75 ZEL k_a . Flash-photolysis. Resonance-absorption.	EX	240-300	(4.8±1.2)(10)	0	0	2	
81 NEL/MAR k_a . M = Ar. Flash-photolysis. Resonance-fluorescence at P(Total) = (10-50) torr. Laser-absorption at P(Total) = 10 torr.	EX	295	(4.94±1.08)(10)			2	
82 MAR/JOH ²⁾ n = 0 assumed.	EX	218-363	(9.15±2.59)(9)	0	-644±79	2	
82 MAR/JOH ²⁾ The preexponential factor expressed as: $A(T/298)^{-2.29}$.	EX	218-363	(8.14±0.30)(10)	-2.29	0	2	
²⁾ k_a . Flash-photolysis. Resonance-fluorescence. OH generated by Flash-photolysis of HONO ₂ . P(Ar) = (10-50) torr. P-independent k.							
82 MAR/WAT ³⁾	EX	228	1.84(11)			2	
82 MAR/WAT ³⁾	EX	246	1.26(11)			2	
82 MAR/WAT ³⁾	EX	298	7.17(10)			2	
82 MAR/WAT ³⁾	EX	415	4.76(10)			2	
³⁾ k_a . M = He. Flash-photolysis. Resonance-fluorescence. OH generated by reacting H with NO ₂ . P = 40 torr. [HONO ₂] = (0.6-8.0) × 10 ¹⁵ molec.cm ⁻³ . Other k's, for the same temperatures as above, but at different pressures in the (0-300) torr. range, are also given. The P-dependence is weaker above 298 K, but stronger below 298 K. The addition complex of channel (c) is considered by the authors as the precursor of channel (a).							
81 WIN/RAV $k_a + k_b$. HONO ₂ /Ar (or SF ₆) flash-photolysis. Resonance-fluorescence. P = (13-60) torr.	EX	224-366	(9.15±2.29)(9)	0	-649±69	2	
82 JOU/POU $k_a + k_b$. Discharge-flow-EPR. OH produced by reacting H with NO ₂ in excess. At 298 K only channel (a) occurs. P = (0.6-2.3) torr. [OH] ₀ = (0.1-7.0) × 10 ¹⁰ molec.cm ⁻³ .	EX	251-403	(4.40±1.20)(9)	0	-876±85	2	
82 KUR/COR $k_a + k_b$. Flash-photolysis of HONO ₂ . [HONO ₂] = (10-221) torr.	EX	225-296	(6.32±2.41)(9)	0	-759±100	2	
82 RAV/EIS ⁴⁾ $k_a + k_b$. M = N ₂ . P(N ₂) = 50 torr.	EX	251	(1.17±0.14)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 RAV/EIS ⁴⁾ $k_a + k_b$. M = SF ₆ . P(SF ₆) = 60 torr.	EX	251	(1.26±0.10)(11)			2	
82 RAV/EIS ⁴⁾ $k_a + k_b$. M = Ar. P(Ar) = 50 torr.	EX	298	(7.53±0.78)(10)			2	
82 RAV/EIS ⁴⁾ $k_a + k_b$. M = SF ₆ . P(SF ₆) = 60 torr.	EX	298	(8.37±1.69)(10)			2	
82 RAV/EIS ⁴⁾ $k_a + k_b$. M = SF ₆ .	EX	220-380	(9.15±2.29)(9)	0	-649±69	2	
⁴⁾ Pulsed Laser-photolysis of HONO ₂ in Ar, N ₂ , or SF ₆ . Channel (a) is the major pathway.							
OH + HO₂NO₂ → H₂O + O₂ + NO₂ (a)							
 → H₂O₂ + NO₃ (b)							
 → HO₂ + HONO₂ (c)							
Hydroxyl + Peroxynitric acid							
80 LIT k_a . Infrared Absorption Spectroscopy.	EX	263-283	(1.75±0.60)(12)	0	0	2	
82 BAR/BAS k_a . Reaction of OH with HO ₂ NO ₂ in a glass- cylinder. FTIR Spectroscopy. OH produced by the reaction: HO ₂ + NO ₂ → OH + NO ₃ . Supersedes 81 BAR/BAS.	EX	295	(2.47±0.60)(12)			2	
82 TRE/BLA ¹⁾ $k_a + k_b + k_c$.	EX	246-324	(4.84±3.43)(12)	0	193±194	2	
82 TRE/BLA ¹⁾ $k_a + k_b + k_c$. B = 0 assumed. (Recommended k.)	EX	246-324	(2.41±0.96)(12)	0	0	2	
¹⁾ OH generated by reacting O(¹ D) with either H ₂ , or or H ₂ O. O(¹ D) obtained by Flash-photolysis of O ₃ .							
OH + CO → H + CO₂ (a)							
 → any other products (b)							
Hydroxyl + Carbon monoxide							
71 BRA/BEL1 k_a . M = Ar.	EX	1300-1900	4.2(11)	0	503±101	2	1.95
71 IZO/KIS k_a . Shock waves. Best data-fit. Total conc. = 5x10 ¹⁷ molec.cm ⁻³ .	DE	1400-2200	9.03(11)	0	503	2	
72 DIX ¹⁾	ES	1050	(2.4±0.12)(11)			2	
72 DIX ¹⁾ Combination of present and other data.	SE	298-1330	3.09(11)	0	370±100	2	1.41
¹⁾ k_a . Fuel-rich H ₂ /N ₂ /O ₂ flames.							
72 STU/NIK1 k_a . M = He (20 Torr).	EX	298	8.13(10)			2	1.15

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _a units	k err. factor
73 DAY/THO k _a . Fuel-rich H ₂ /N ₂ /O ₂ flame k.	ES	1050	(2.4±0.12)(11)			2	
73 GAR/MAL k _a . M = Ar. Data-fit to a proposed mechanism.	EX	1200-2500	4.0(12)	0	4026	2	1.25
73 PEE/MAH1 k _a . Lean CH ₄ /O ₂ flames.	ES	1750	2.8(11)			2	
73 PEE/MAH1 k _a . Lean CH ₄ /O ₂ flames.	ES	1600-1900	1.36(12)	0	2768±101	2	
73 SMI/ZEL1 k _a . Within the 210-460 K range, slight positive T-dependence, possibly curved.	EX	300	8.7(10)			2	
73 WES/DEH1 k _a . Nonlinear Arrhenius behaviour. From 298 to 915 K, k increases from 8x10 ¹⁰ to 13.1x10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ .	EX	298	8.0(10)			2	
74 DAV/FIS k _a . M = He.	EX	220-373	(1.29±0.11)(11)	0	81±40	2	
74 HOW/EVE k _a . M = He, Ar, or N ₂ .	EX	296	9.40(10)			2	
74 TRA/ROS2 k _a . M = Ar. CO ₂ is vibrationally excited.	EX	300	7.53(10)			2	
75 BIO/LAZ k _a . Uninhibited CH ₄ /O ₂ /Ar flame.	EX	1250-1750	4.7(11)	0	0	2	
75 CAM/HAN1 k _a /k _{ref} . Estimated ratio. k _{ref} : OH + NO ₂ (+ M) → HNO ₃ (+ M).	RL	292	(5.3±1.0)(-2)			2/2	
75 GOR/MUL1 k _a . M=Ar (710 torr.) + H ₂ O (10 torr.) + CO (10 torr.)	EX	298	(9.07±0.05)(10)			2	
75 STE/ZEL k _a . Nonlinear Arrhenius behaviour. For 300-900 K: log k = (10.85±0.08 + 4.0x10 ⁻⁴ T (cm ³ mol ⁻¹ s ⁻¹ .)	EX	300	9.33(10)			2	1.20
75 TRA/ROS k _a . M = Ar. CO ₂ is vibrationally excited.	EX	300	7.53(10)			2	
75 VAN/PEE k _a . Lean CO/H ₂ /O ₂ flame. Non-linear Arrhenius behaviour. k increases slightly from 400 to 800 K.	EX	400	8.0(10)			2	
75 VAN/PEE k _a . Lean CO/OH ₂ /O ₂ flame. log k = (10.85±0.08) + 4.0x10 ⁻⁴ T cm ³ mol ⁻¹ s ⁻¹ .	EX	1000-1800	2.32(12)	0	2869	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 ZEL k_a . Flash -photolysis. Resonance-absorption. 2) $k = 6.76 \times 10^{10} \exp(8.7 \times 10^{-4} T) \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. (Empirical expression).	EX	220-900	2)	2)	2)	2	2.0
76 ATK/PER2 k_a . M = Ar. P = (25-634) torr. Limiting high-pressure k.	EX	299	(9.28±0.96)(10)			2	
76 BRA/CAP k_a/k_{ref} . k_{ref} : OH + CH ₄ → H ₂ O + CH ₃	RL	1300	1.8(-1)			2/2	
76 COX/DER1 k_a/k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H.	RL	298	(3.86±0.34)(1)			2/2	
76 COX/DER1 k_a .	ES	298	(1.63±0.12)(11)			2	
76 SIE/SIM1 k_a/k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H. Limiting high-pressure ratio.	RL	217-298	2.0(-1)	0	-1711	2/2	
76 SIE/SIM1 k_a/k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H. Rate ratio increasing from a limiting low-pressure value of 14 to a limiting high-pressure value of 50.	RL	298	1.4(1)			2/2	
77 ATR/BAL ³⁾ k_a/k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H.	RL	773	(2.35±0.20)(-1)			2/2	
77 ATR/BAL ³⁾ k_a .	RN	773	9.6(10)			2	
³⁾ Aged boric-acid coated vessel. P(Total) = 500 torr.							
77 CHA/USE ⁴⁾ k_a/k_{ref} . P = 100 torr.	RL	298	(5.86±0.84)(-2)			2/2	
77 CHA/USE ⁴⁾ k_a . P = 100 torr.	RN	298	(8.28±1.18)(10)			2	
77 CHA/USE ⁴⁾ k_a/k_{ref} . P = 700 torr.	RL	298	(1.27±0.07)(-1)			2/2	
77 CHA/USE ⁴⁾ k_a . P = 700 torr.	RN	298	(1.79±0.98)(10)			2	
⁴⁾ k_{ref} : OH + (CH ₃) ₃ CH → H ₂ O + (CH ₃) ₃ C (a) → H ₂ O + (CH ₃) ₂ CHCH ₂ (b)							
77 OVE/PAR1 ⁵⁾ k_a . M = He. P = 50 torr.	EX	296	(1.22±0.05)(11)			2	
77 OVE/PAR1 ⁵⁾ k_a . M = SF ₆ . P = (200-350) torr.	EX	296	(1.95±0.12)(11)			2	
⁵⁾ Limiting high-pressure k.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 BIE/ZET2 ⁶⁾ k _a . P(He, or N ₂) < 50 torr.	EX	297	9.03(10)			2	
78 BIE/ZET2 ⁶⁾ k _a . P(He) = 740 torr.	EX	297	(1.20±0.22)(11)			2	
78 BIE/ZET2 ⁶⁾ k _a . P(N ₂) = 740 torr.	EX	297	(1.38±0.20)(11)			2	
78 BIE/ZET2 ⁶⁾ k _a . P(N ₂) = 745 torr.	EX	297	(1.70±0.17)(11)			2	
78 BIE/ZET2 ⁶⁾ k _a . P(N ₂) = 750 torr.	EX	297	(8.67±1.26)(10)			2	
⁶⁾ k dependent on pressure and purity-degree of M. UV-Photolysis. Resonance-absorption.							
78 BUT/SOL k _a . Quartz reactor. H ₂ O ₂ photolysis. Gas-chromatography. P(O ₂ + N ₂) = (100-600) torr.	EX	305	(1.62±0.24)(11)			2	
79 CLY/HOL k _a . Resonance-fluorescence. Gas-chromatography.	EX	293-430	1.32(11)	0	88±40	2	1.3
79 ZEL k _a . ⁷⁾ k = exp(24.98+9.2x10 ⁻⁴ T) cm ³ mol ⁻¹ s ⁻¹ . Non-Arrhenius best-fit of all data. Critical evaluation.	EX	300-2000	⁷⁾	⁷⁾	⁷⁾	2	
77 PER/ATK2 ⁹⁾ k _{overall} .	EX	299	⁸⁾			2	
⁸⁾ k dependent on the nature and pressure of the third body. For M = Ar: k = (9.03±0.90)x10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ at 25.5 torr. increasing to k = (9.76±1.45)x10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ at 643.3 torr. For M = SF ₆ : k = (9.22±0.96)x10 ¹⁰ cm ³ mol ⁻¹ s ⁻¹ at 25.3 torr. increasing to k = (2.07±0.21)x10 ¹¹ cm ³ mol ⁻¹ s ⁻¹ at 603.5 torr. The assumed mechanism (73 SMI/ZEL) is: OH + CO → HOCO [†] (a) HOCO [†] → OH + CO (-a) HOCO [†] → H + CO ₂ (b) HOCO [†] + M → HOCO + M (c) (with HOCO [†] removed by O ₂) Steady-state treatment gives: k = k _a (k _b + k _c [M]) / (k _a + k _b + k _c [M])							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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From this expression and the experimental data,
estimates of individual rate constants and ratios
obtained are:

$$k_a = 3.61 \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1};$$

$$k_{-a} \sim 8 \times 10^9 \text{ s}^{-1};$$

$$k_b \sim 3 \times 10^9 \text{ s}^{-1};$$

$$k_c \sim 2.41 \times 10^{14} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1};$$

$$k_b / (k_{-a} + k_b) = 0.25;$$

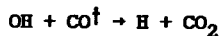
$$k_c / (k_{-a} + k_b) = 2.41 \times 10^4 \text{ cm}^3 \text{ mol}^{-1}.$$

9) Flash-photolysis of H₂O vapor.

Resonance-Fluorescence.

$$P(\text{Total}) = (25-643) \text{ torr.}$$

M = Ar, or SF₆.



Hydroxyl + Carbon monoxide

81 DRE/WOL ¹⁾ EX 298 (9.1±3.4)(10) 2

$$T_t = T_r = T_v = 298\text{K.}$$

81 DRE/WOL ¹⁾ EX 298 (8.2±3.0)(10) 2

$$T_t = T_r = 298\text{K. } T_v = 1400\text{K.}$$

81 DRE/WOL ¹⁾ EX 298 (7.8±2.9)(10) 2

$$T_t = T_r = 298\text{K. } T_v = 1800\text{K.}$$

¹⁾ Discharge-flow.

IR-resonance radiation.



Hydroxyl-d + Carbon monoxide

82 PAR/IRW ²⁾ EX 298 (3.12±0.30)(10) 2

$$M = \text{He. } P(\text{He}) = 20 \text{ torr.}$$

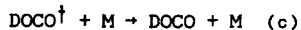
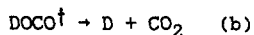
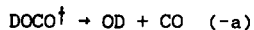
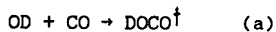
82 PAR/IRW ²⁾ EX 298 (1.03±0.15)(11) 2

$$M = \text{N}_2. P(\text{N}_2) = 650 \text{ torr.}$$

82 PAR/IRW ²⁾ EX 298 (1.07±0.07)(11) 2

$$M = \text{CF}_4, \text{ or SF}_6. P(\text{CF}_4, \text{ or SF}_6) = 600 \text{ torr.}$$

¹⁾ The assumed mechanism (73 SMI/ZEL) is:



(with DOCO[†] removed by O₂, or a radical)

Steady-state treatment gives:

$$k = k_a(k_b + k_c[M]) / (k_{-a} + k_b + k_c[M]).$$

From this expression and the experimental data, individual rate constants and ratios obtained are:

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$k_a = (1.37 \pm 0.16) \times 10^{11} \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$. M = CF ₄ , or N ₂ . Average k. $k_{-a} \approx 8.4 \times 10^8 \text{ s}^{-1}$. (Estimated k) $k_b \approx 1.9 \times 10^8 \text{ s}^{-1}$. (Estimated k) $k_{-a}/k_b = (4.4 \pm 0.7)$ M = CF ₄ , or N ₂ . Average ratio. $k_c/k_b = (4.3 \pm 1.4) \times 10^5$, for M = CF ₄ $= (4.7 \pm 1.4) \times 10^5$, for M = N ₂ $= (1.4 \pm 0.6) \times 10^5$, for M = He.						
2) Flash-photolysis of D ₂ O vapor in Vacuum-UV. Time-resolved Resonance-Absorption. [CO] = $3.0 \times 10^{11} \text{ molec. cm}^{-3}$. P = (20-650) torr. Supersedes 81 PAR/IRW.						
OH(v=1) + CO → H + CO₂ Hydroxyl + Carbon monoxide						
77 SPE/END	EX	295	≤1.81(11)			2
77 SPE/GLA	EX	295	<3.01(12)			2
OH(v=9) + CO₂ → products Hydroxyl + Carbon dioxide						
72 WOR/COL	EX	298	(1.45 ± 0.60)(10)			2
OH + CH₃ → H + H + HCHO (a) OH + CH₃ → CH₃OH (b) Hydroxyl + Methyl						
80 BHA/FRA	EX	1700-2300	2.0(16)	0	13860	2
k_a . Shock-tube. Resonance-Absorption.						
81 TSU/KAT ¹⁾	RN	1500-1900	8.32(9)	0	9863	2
Total conc. = $6.0 \times 10^{18} \text{ molec. cm}^{-3}$.						
81 TSU/KAT ¹⁾	RN	1500-1900	4.90(10)	0	9382	2
Total conc. = $3.0 \times 10^{19} \text{ molec. cm}^{-3}$.						
81 TSU/KAT ¹⁾	DE	1500-1900	1.20(11)	0	8781	2
Total conc. = $6.0 \times 10^{19} \text{ molec. cm}^{-3}$.						
1) k_b . M = Ar. CH ₃ OH/O ₂ thermal oxidation behind reflected shock-waves. $k_1 = k_{-1}K$. Same data given in 81 TSU/HAS.						
80 SWO/HOC	EX	296	(5.6 ± 1.5)(13)			2
k_{overall} . Flash-photolysis of H ₂ O vapor. P ~ 760 torr. M = N ₂ , H ₂ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₄ → H₂O + CH₃						
Hydroxyl + Methane						
71 BAK/BAL Rate constant per CH bond.	CO	298-753	6.3(12)	0	2516	2
73 PEE/MAH1	EX	1100-1900	3.0(13)	0	3020	2
74 DAV/FIS	EX	240-373	(1.42±0.13)(12)	0	1711±88	2
74 MAR/KAU	EX	290-440	(2.31±0.12)(12)	0	1842±20	2
75 GOR/MUL1 ¹⁾	EX	381	(1.57±0.16)(10)			2
75 GOR/MUL1 ¹⁾	EX	416	(3.3±0.1)(10)			2
¹⁾ In an atmosphere of H ₂ O vapor.						
75 OVE/PAR	EX	295	(3.92±0.16)(9)			2
75 STE/ZEL	EX	300-700	2.8(12)	0	1862	2
76 COX/DER1 k _{ref} : OH + H ₂ → H ₂ O + H.	RL	298	(1.04±0.12)			2/2
76 COX/DER1	ES	298	(4.58±0.12)(9)			2
76 HCW/EVE1	EX	296	(5.72±0.84)(9)			2
76 ZEL/STE Flash-photolysis. Resonance-absorption. The exponential factor expressed as: A(T/298) ^{3.08} . Same data given in 75 ZEL.	EX	300-900	1.45(11)	3.08	1010	2 1.15
78 ERN/WAG ²⁾	EX	1300	(2.5±0.8)(12)			2
78 ERN/WAG ²⁾ Empirical fit. The preexponential factor expressed as: A(T/298) ^{2.13} .	EX	250-2000	2.89(11)	2.13	1234	2
²⁾ Flash-photolysis-Shock-tube technique.						
78 SHA The preexponential factor expressed as: A(T/298) ² .	CO	300-2500	7.56(11)	2.0	1485	2
79 ZEL Critical evaluation. The preexponential factor expressed as: A(T/298) ^{2.13}	SE	300-2000	2.89(11)	2.13	1233	2
80 SWO/HOC Flash-photolysis of H ₂ O vapor. P ~ 760 torr.	EX	296	(4.2±0.4)(9)			2
80 TUL/RAV ³⁾ Best-fit non-linear Arrhenius expression. The preexponential factor expressed as: A(T/298) ^{1.92} .	EX	298-1020	4.48(11)	1.92	1355	2
80 TUL/RAV ³⁾ ³⁾ M = Ar. Flash-photolysis. Resonance-fluorescence. P(H ₂ O) = 150 mtorr. P(CH ₄) = 0-1 torr. P(Ar) = 50 torr.	EX	298	(4.52±0.36)(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 FAI/SMI ⁴)	EX	830	(7.53±2.71)(11)			2
82 FAI/SMI ⁴)	EX	1030	(7.82±2.41)(11)			2
82 FAI/SMI ⁴)	EX	1400	(2.59±0.60)(12)			2
⁴) Two-laser method for real-time measurement of radical-molecule k's. OH generated by irradiation of a SF ₆ /N ₂ /H ₂ O ₂ /H ₂ O mixture at 40 torr., by a pulsed IR CO ₂ laser.						
82 JEO/KAU1 ⁵)	EX	269-473	(3.37±0.90)(12)	0	1973±101	2
82 JEO/KAU1 ⁵)	EX	269-473	3.36(11)	2.0	1263	2
Modified, non-linear Arrhenius expression. Optimized. The preexponential factor expressed as: A(T/298) ² .						
⁵) Discharge-flow. Resonance-fluorescence. [CH ₄] = (0.23-8.85)×10 ¹⁵ molec.cm ⁻³ .						
OH(v=n) + CH ₄ → H ₂ O + CH ₃						
Hydroxyl + Methane						
72 WOR/COL	EX	298	(8.43±1.20)(9)			2
Unreported T assumed to be 298K.						
77 SPE/END	EX	295	≤1.81(10)			2
Upper-limit k.						
OH + CDH ₃ → H ₂ O + CDH ₂ (a) → HDO + CH ₃ (b)						
Hydroxyl + Methane-d						
75 GOR/MUL1	EX	416	(2.2±0.1)(10)			2
k _a + k _b . In an atmosphere of water vapor.						
OH + CD ₂ H ₂ → H ₂ O + CD ₂ H (a) → HDO + CDH ₂ (b)						
Hydroxyl + Methane-d ₂						
75 GOR/MUL1	EX	416	(1.8±0.1)(10)			2
k _a + k _b . In n atmosphere of water vapor.						
OH + CD ₃ H → H ₂ O + CD ₃ (a) → DHO + CD ₂ H (b)						
Hydroxyl + Methane-d ₃						
75 GOR/MUL1	EX	416	(6.7±0.3)(9)			2
k _a + k _b . In an atmosphere of water vapor.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
OH + CD ₄ → DHO + CD ₃ Hydroxyl + Methane-d ₄						
75 GOR/MUL1 In an atmosphere of H ₂ O vapor.	EX	416	(3.0±1.0)(9)			2
OH + HCHO → H ₂ O + CHO (a) → H ₂ O + CHO [†] (b) → HCOOH + H (c)						
Hydroxyl + Formaldehyde						
71 MOR/NIK1 k _a .	EX	298	8.43(12)			2 1.25
71 MOR/NIK2 k _a . k _{ref} : OH + CH ₃ CH=CH ₂ → products.	EX	300	9.0(-1)			2/2
73 PEE/MAH1 k _a .	ES	1400-1800	≈2.3(13)	0	0	2
77 VAN/VAN k _a .	ES	300-1600	3.9(13)	0	705	2
78 NIK/MAK ¹⁾ k _a /k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(1.5±0.1)			2/2
78 NIK/MAK ¹⁾ k _a .	RN	298	9.03(12)			2
¹⁾ HCHO + HONO photolysis. FTIR-spectroscopy.						
78 ATK/PIT3 k _a . Flash-photolysis. Resonance-fluorescence.	EX	299-426	7.53(12)	0	88±151	2
80 STI/NAV k _a + k _c . Flash-photolysis. Resonance-fluorescence. T-, and P-flash-intensity independent.	EX	228-362	(6.32±0.66)(12)	0	0	2
78 HOR/SU k _b /k _c . HCHO photolysis at 313 nm. P(HCHO) = 8 torr. P(O ₂) = (0.02-8) torr. P(CO ₂) = (0-300) torr.	RL	298	≈5.0(-1)			2/2
80 MOR/HEI k _b /(k _a + k _b + k _c). NO ₂ Photolysis at 366 nm., in presence of HCHO. IR absorption spectroscopy. k _{ref} : OH + HCHO → products.	RL	296	(4.9±1.6)(-1)			2/2
78 SMI k _{overall} . Discharge-flow. Mass-spectrometry. k shows no significant trends when the [HCHO] and [OH] are varied by factors of 8 and 4, respectively, at 298 and 334 K. E _a = 1434±478 cal.mol ⁻¹ between 268 and 334 K.	RN	298	(3.91±0.90)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + HCOOH → products						
Hydroxyl + Formic acid						
82 ZET/STU Pulsed Vacuum UV-photolysis of H ₂ O, Ar and HCOOH mixtures. Resonance-fluorescence. P(H ₂ O) = (0.03-0.2) torr. P(Ar) = (25-100) torr.	EX	298	(1.93±0.12)(11)			2
OH + CH₃OH → H₂O + CH₂OH (a) → H₂O + CH₃O (b)						
Hydroxyl + Methanol						
75 OSI/SIM (k _a + k _b)/k _{ref} . k _{ref} : OH + CO → H + CO ₂	RL	298	(6.3±1.0)(-1)			2/2
75 OSI/SIM (k _a + k _b)/k _{ref} . k _{ref} : OH + CO → H + CO ₂	RL	345	(9.8±2.0)(-1)			2/2
76 CAM/MCL k _a + k _b .	EX	292	(5.7±0.6)(11)			2
75 BOW2 k _a . M = Ar. Reflected shock waves. Best data-fit. [Ar] = (5.7-17.0)×10 ¹⁸ molec.cm ⁻³ . [CH ₃ OH] = 1.3×10 ¹⁷ molec.cm ⁻³ . [O ₂] = 2.5×10 ¹⁷ molec.cm ⁻³ .	ES	1545-2180	3.0(13)	0	3000	2
78 OVE/PAR1 k _a . Flash-photolysis. Resonance-absorption.	EX	296	(6.4±0.6)(11)			2
78 RAV/DAV k _a + k _b . Flash-photolysis. Resonance-fluorescence. P(CH ₃ OH) = 10 torr.	EX	298	(6.02±0.60)(11)			2
81 TSU/HAS k _a . M = Ar, CH ₃ OH/O ₂ thermal oxidation in Ar, behind reflected shock-waves.	ES	1200-1800	2.0(14)	0	3007	2
81 VAN/VAN k _a . CH ₃ OH/O ₂ burned at 40 torr., with or without added Ar or H ₂ . Molecular beam-sampling.	DE	1000-2000	4.8(13)	0	2265	2
OH + CS₂ → SH + COS (a) → SOH + CS (b)						
Hydroxyl + Carbon disulfide						
80 COX/SHE ¹⁾ k _a /k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(6.0±2.0)(-2)			2/2
80 COX/SHE ¹⁾ k _a .	RN	297	(2.59±0.96)(11)			2
¹⁾ Photolysis of HONO and CS ₂ . Gas-chromatography. P = 760 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 IYE/ROW k _a . Photolysis of H ₂ O ₂ + CS ₂ mixtures. Gas-chromatography. Upper-limit k.	EX	298	<1.81(9)			2
82 LEU/SMI2 ²⁾ k _a .	EX	298	≤4.22(9)			2
82 LEU/SMI2 ²⁾ k _a . ²⁾ Discharge-flow Resonance-fluorescence. OH generated by reacting H with NO ₂ . Upper-limit k's. P-independent in the (2.2-58) torr. range. [CS ₂] ₀ = (0.4-35.1) × 10 ¹⁵ molec.cm ⁻³ . [OH] ₀ = (0.7-3.7) × 10 ¹¹ molec.cm ⁻³ .	EX	520	≤1.81(9)			2
78 ATK/PER1 k _a + k _b . Upper-limit k.	EX	300-425	<4.22(10)			2
78 KUR2 k _a + k _b . Flash-photolysis. Resonance-fluorescence. Channel (a) is more probable than (b).	EX	296	(1.11±0.20)(11)			2
80 WIN/SHA ³⁾ k _a + k _b .	EX	251	<5.96(9)			2
80 WIN/SHA ³⁾ k _a + k _b .	EX	297	<9.03(8)			2
80 WIN/SHA ³⁾ k _a + k _b .	EX	363	<9.64(8)			2
³⁾ Flash-photolysis. Resonance-fluorescence. M = Ar, or SF ₆ . Upper-limit k's. P(H ₂ O) = (230-250) mtorr. P = (35-50) torr.						
82 BIE/HAR k _a + k _b . Discharge-flow. OH generated by reacting H with NO ₂ . Upper-limit k. [OH] ₀ = (0.2-2.0) × 10 ¹² molec.cm ⁻³ . P (Total) ~ 2 torr. (He)	EX	298	≤3.01(10)			2
82 JON/BUR k _a /k _b . CS ₂ /HONO photolysis in N ₂ (or N ₂ /O ₂). COS is the principal product. P(O ₂) = (40-380) torr.	EX	295	(1.02±0.54)(12)			2
OH + COS → SH + CO ₂ (a) → SOH + CO (b)						
Hydroxyl + Carbon oxide sulfide						
80 COX/SHE ¹⁾ k _a /k _{ref} . Upper-limit ratio. k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	≤5.0(-3)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 COX/SHE ¹⁾ k _a . Upper-limit k.	RN	297	≤2.41(10)			2
1) Photolysis of HONO and COS. Gas-chromatography. P(O ₂) = (40-380) torr. P = 760 torr.						
78 ATK/PER1 k _a + k _b . Upper-limit k.	EX	299-430	<4.22(9)			2
78 KUR2 k _a + k _b . Flash-photolysis. Resonance-fluorescence.	EX	296	(3.41±0.73)(10)			2
80 RAV/KRE k _a + k _b . Laser-photolysis of Nitric acid. Flas-photolysis. Resonance-fluorescence. Upper-limit k.	EX	298	≤5.30(9)			2
81 LEU/SMI k _a + k _b . Discharge-flow. Resonance-fluorescence.	EX	300-520	(7.83±1.81)(11)	0	2300±100	2
OH(v=9) + COS → products						
Hydroxyl + Carbon oxide sulfide						
72 WOR/COL	EX	298	(1.51±0.90)(10)			2
OH + CH₃SH → products						
Hydroxyl + Methanethiol (Methylmercaptan)						
77 ATK/PER4 ¹⁾	EX	299-426	5.35(12)	0	-398±151	2
77 ATK/PER4 ¹⁾	EX	299-426	(2.04±0.20)(13)	0	0	2
1) Flash-photolysis. Resonance-fluorescence.						
80 COX/SHE ²⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(1.13±0.11)(-1)			2/2
80 COX/SHE ²⁾	RN	297	(5.44±0.51)(13)			2
2) Photolysis of HONO and CH ₃ SH. Gas-chromatography. P = 760 torr.						
81 WIN/KRE H ₂ O/Ar/CH ₃ SH flash-photolysis. Resonance-fluorescence. P(H ₂ O) = (0.05-0.15) torr. P(Ar) = (40-120) torr.	EX	244-367	(6.93±2.35)(12)	0	-338±100	2
OH + CN → H + NCO						
Hydroxyl + Cyanogen						
76 MOR Premixed flames. T-independent k. E _a = 0 assumed.	EX	2300-2560	6.03(13)	0	0	2
77 HAY2 Fuel-rich flames.	EX	1950-2380	(5.6±0.7)(13)	0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + HCN → H + HOCN (a)						
→ H ₂ O + CN (b)						
Hydroxyl + Hydrocyanic acid						
77 HAY2	EX	1950-2380	(2.0±0.2)(11)	0	0	2
k _a . Fuel-rich flames.						
79 PHI2	EX	298-563	(3.23±0.65)(10)	-1.0	1860	2
k _b . Discharge-flow. Resonance-fluorescence.						
The preexponential factor expressed as:						
A(T/298) ⁻¹ .						
P >10 torr.						
OH + CH₃NH₂ → products						
Hydroxyl + Methanamine						
77 ATK/PER4 ¹)	EX	299-426	6.14(12)	0	-229±151	2
77 ATK/PER4 ¹)	EX	298	(1.33±0.13)(12)			2
¹) Flash-photolysis.						
Resonance-fluorescence.						
OH + NH₂NHCH₃ → products						
Hydroxyl + Hydrazine, methyl-						
79 HAR/ATK	EX	298-424	(3.91±0.79)(13)	0	0	2
M = Ar. Flash-photolysis.						
Resonance-fluorescence.						
P(Ar) = (25-50) torr.						
OH + CH₃ONO → products						
Hydroxyl + Nitrous acid methyl ester (Methyl nitrite)						
75 CAM/GOO2	ES	292	(8.0±1.1)(11)			2
82 AUD/BAU1	EX	295	(7.1±1.2)(11)			2
Static system. OH generated by the chain reaction:						
H ₂ O ₂ + NO ₂ + CO.						
P < 75 torr. [CO] ₀ ~ 3.0x10 ¹⁸ molec.cm ⁻³ .						
[CH ₃ ONO] ₀ < 3.6x10 ¹⁷ molec.cm ⁻³ .						
[H ₂ O ₂] ₀ ~ 9.0x10 ¹⁵ molec.cm ⁻³ .						
[NO ₂] ₀ ~ 3.3x10 ¹⁶ molec.cm ⁻³ .						
OH + CH₃NO₂ → products						
Hydroxyl + Methane, nitro-						
75 CAM/GOO2	ES	292	(5.5±0.6)(11)			2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH=CH → H + CH ₂ =C=O (a)						
→ H ₂ + CH=C=O (b)						
→ CO + CH ₃ (c)						
→ H + CH=COH (d)						
→ [HO, CH=CH] ⁺ (e)						
Hydroxyl + Ethyne						
77 PER/ATK2	EX	288-422	1.15(12)	0	312±201	2
k _a (or, more likely, k _d .) M = Ar. P > 200 torr.						
77 VAN/VAN	ES	570-850	3.2(11)	0	101	2
k _a . M = O ₂ , or O ₂ + Ar.						
80 BAR/DOV	EX	2650	1.81(12)			2
k _a . Ethyne oxidation by water vapor behind shock-waves. Time-of-flight Mass-spectrometry. It is assumed that step (a) is followed by the fast dissociation of CH ₂ =C=O into CH ₂ and CO.						
82 BIT/HOW	EX	1700-1900	(1.3±0.3)(12)	0	0	2
k _a . C ₆ H ₆ /O ₂ /Ar flame. Molecular beam Mass-spectrometry. P = 20 torr.						
71 BRE/GLA	EX	295	(1.14±0.36)(11)			2
k _b . Channel (b) is preferable to the possible abstraction path: OH + CH=CH → H ₂ O + CH=C						
77 VAN/VAN	ES	650-1110	5.5(13)	0	6895	2
k _c . M = O ₂ , or O ₂ + Ar.						
81 TSU/KAT	ES	1500-1900	2.0(13)	0	1564	2
k _c . CH ₃ OH/O ₂ thermal oxidation in Ar, behind reflected shock-waves. UV-absorption. IR-emission. Same data given in 81 TSU/HAS.						
73 SMI/ZEL1	EX	210-460	1.2(12)	0	253	2
k _a + k _b + k _c . M = He.						
74 PAS/CAR1	EX	298	(1.20±0.36)(11)			2
k _a + k _b + k _c . M = He.						
75 DAV/FIS	EX	300	(9.94±0.90)(10)			2
k _a + k _b + k _c . M = He. Channel (a) gives probably the primary products. P-independent k.						
74 PAS/CAR2	EX	298	(1.76±0.16)(11)			2
k _a + k _b + k _c . Discharge-flow. P ~ 1 torr.						
77 DAV	EX	298	(9.94±0.90)(10)			2
k _a + k _b + k _c . Channel (a) is probably predominant. M = He. Flash-photolysis. Resonance-fluorescence. P(He) = (20-500) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 GOR/MUL1 k_a . In an atmosphere of water vapor.	EX	381	(3.75±0.20)(12)			2
75 GOR/MUL1 k_a . In an atmosphere of water vapor.	EX	416	(4.4±0.2)(12)			2
75 PAS/CAR Rate constant expressed as nk_a , where n is a stoichiometric factor.	EX	300	(1.39±0.08)(12)			2
76 HOW k_a . M = He. Limiting high-pressure k.	EX	296	2.41(12)			2
76 LLO/DAR2 k_a/k_{ref} . k_{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	305	2.88			2/2
76 LLO/DAR2 k_a .	RN	305	(5.2±1.0)(12)			2
77 ATK/PER2 ²⁾	EX	299-425	1.3(12)	0	-388±151	2
77 ATK/PER2 ²⁾	EX	299	(4.73±0.48)(12)			2
²⁾ k_a . M = Ar. Limiting high-pressure k.						
77 DAV ³⁾	EX	298	(2.19±0.12)(12)			2
M = N ₂ . P(N ₂) = 3 torr.						
77 DAV ³⁾	EX	298	(1.35±0.13)(12)			2
M = He. P(He) = 3 torr.						
77 DAV ³⁾	EX	298	(3.21±0.39)(12)			2
M = He. P(He) = 300 torr.						
³⁾ k_a . Flash-photolysis. Resonance-fluorescence.						
77 OVE/PAR2 k_a . M = H ₂ O, SF ₆ , CF ₄ . Limiting high-pressure k.	EX	296	(6.0±1.0)(12)			2
78 OVE/PAR2 ⁴⁾	EX	298	(5.4±0.5)(12)			2
k_a . M = He. P(He) = 50 torr.						
78 OVE/PAR2 ⁴⁾	EX	298	(6.5±0.5)(12)			2
k_a . M = SF ₆ , or CF ₄ . P(SF ₆ , or CF ₄) = 400 torr.						
⁴⁾ Vacuum UV photolysis of H ₂ O.						
78 PRE k_a . Laser Magnetic Resonance Spectrometry.	EX	293	(4.7±1.5)(11)			2
80 COX k_a . HONO photosensitized oxidation in synthetic air. Gas-chromatography. [HONO] = (3-20) ppm. [NO] = NO ₂] = (0.3-3.0) ppm.	SE	300	4.82(12)			2
80 FAR/SMI k_a . M = He. Discharge flow. Resonance-fluorescence. Mass-spectrometry.	EX	298	(1.12±0.18)(19)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC2 ⁵⁾ k _a k _{ref} . k _{ref} : OH +  + products.	RL	299	(1.12±0.05)			2/2
82 ATK/ASC2 ⁵⁾ k _a . ⁵⁾ CH ₃ ONO/NO/CH ₂ =CH ₂ and Cyclohexane photolysis. [CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ . [CH ₂ =CH ₂] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . [NO] ₀ ~ 1.19×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(5.11±0.23)(12)			2
76 BRA/CAP k _b /k _{ref} . k _{ref} : CH ₄ + OH → CH ₃ + H ₂ O	RL	1300	2.33			2/2
76 MEA/HEI k _b /(k _a + k _b).	RL	298	2.6(-1)			2/2
OH + CD ₂ =CD ₂ → products Hydroxyl + Ethene-d ₄						
78 NIK/MAK k _{ref} : OH + CH ₂ =CH ₂ → products. CD ₂ =CD ₂ /HONO Photolysis. FTIR-Spectroscopy. P(air) = 700 torr.	RL	298	(1.03±0.06)			2
OH + CH ₃ CH ₃ → H ₂ O + CH ₃ CH ₂ Hydroxyl + Ethane						
71 BAK/BAL Rate constant per CH bond.	CO	298-753	1.45(13)	0	1772	2
71 BAK/BAL ¹⁾	RL	753	(1.05±0.11)(1)			2/2
79 BAL/WAL ¹⁾	RL	753-773	1.28	0	-1070	2/2
A and B recalculated from an empirical formula.						
¹⁾ k _{ref} : OH + H ₂ → H ₂ O + H.						
75 GOR/MUL ²⁾	EX	381	(4.0±0.2)(11)			2
75 GOR/MUL ²⁾	EX	416	(4.8±0.3)(11)			2
²⁾ In an atmosphere of water vapor.						
75 HUC/BOO ³⁾	RL	653	(9.6±1.1)			2/2
75 OVE/FAR	EX	295	(1.59±0.10)(11)			2
76 BRA/CAP ³⁾	RL	1300	2.88			2/2
³⁾ k _{ref} : OH + CH ₄ → H ₂ O + CH ₃						
76 HOW/EVE2	EX	296	(1.75±0.36)(11)			2
79 LEU	EX	298	(1.57±0.24)(11)			2
Discharge-flow. Resonance-fluorescence.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 LEE/TAN Discharge-flow. Resonance-fluorescence. OH generated by reacting H with NO ₂ .	EX	295	(1.39±0.24)(11)			2
OH + CH ₂ =C=O → CHO + HCHO Hydroxyl + Ethenone (Ketene)						
77 VAN/VAN	ES	480-1000	2.8(13)	0	0	2
OH + CH ₃ CHO → H ₂ O + CH ₃ CO (a) → H ₂ O + CH ₂ CHO (b) Hydroxyl + Acetaldehyde						
71 MOR/NIK2 k _a + k _b . k _{ref} : CH ₃ CH=CH ₂ + OH → products.	RL	300	9.0(-1)			2/2
71 MOR/STE k _a + k _b . Channel (a) is predominant.	EX	300	9.03(12)			2 1.25
76 COX/DER3 k _a . Upper-limit k.	EX	296	≤1.2(13)			2
78 ATK/PIT3 k _a + k _b . Flash-photolysis. Resonance-fluorescence.	EX	299-426	4.14(12)	0	257±151	2
78 NIK/MAK ¹⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(1.9±0.2)			2/2
78 NIK/MAK ¹⁾ ¹⁾ k _a + k _b . CH ₂ =CH ₂ /HONO photolysis. FTIR-spectroscopy. P(air) = 700 torr.	RN	298	9.64(12)			2
81 KER/SHE ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(1.50±0.50)			2/2
81 KER/SHE ¹⁾ k _a + k _b . ¹⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(7.23±2.41)(12)			2
OH + CH ₃ COOH → products Hydroxyl + Acetic acid						
82 ZET/STU H ₂ O/Ar/CH ₃ COOH photolysis. Resonance-fluores- cence. P(Ar) = (20-500) torr. P(H ₂ O) = 0.1 torr.	EX	298	(3.61±0.72)(11)			2
OH + CH ₃ CH ₂ OH → H ₂ O + CH ₃ CHOH (a) → any other products (b) Hydroxyl + Ethanol						
82 NAT/BHA k _a . M = O ₂ + Ar. Ethanol/O ₂ /Ar ignition behind reflected shock-waves. Data-fit. P = (1-2) atm.	ES	1300-1700	3.00(13)	0	3000	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 CAM/MCL k_{overall}	EX	292	(1.8±0.2)(12)			2
78 OVE/PAR1 k_{overall} . Flash-photolysis. Resonance-fluorescence.	EX	296	(2.25±0.22)(12)			2
78 RAV/DAV k_{overall} . Flash-photolysis. Resonance-fluorescence. P(Ethanol) < 2.5 torr.	EX	298	(1.58±0.22)(12)			2
OH + (CH₃)₂O → H₂O + CH₂OCH₃						
Hydroxyl + Methane, oxybis-						
77 PER/ATK1	EX	299-427	7.77(12)	0	388±151	2
77 PER/ATK1	EX	299	(2.11±0.21)(12)			2
OH + (CH₃)₂S → products						
Hydroxyl + Methane, thiobis-						
78 ATK/PER1 Flash-photolysis. Resonance-fluorescence.	EX	300-427	(3.29±0.72)(12)	0	-179±151	2
78 KUR1 Flash-photolysis. Resonance-fluorescence. Recommended k.	EX	273-426	(3.66±1.53)(12)	0	134±135	2
80 COX/SHE ¹⁾ k_{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(1.14±0.18)			2/2
80 COX/SHE ¹⁾	RN	297	(5.48±0.84)(12)			2
¹⁾ Photolysis of HONO and (CH ₃) ₂ S. P = 760 torr.						
81 WIN/KRE Flash-photolysis of H ₂ O/Ar/(CH ₃) ₂ S mixtures. P(H ₂ O) = (0.05-0.15) torr. P(Ar) = (50-200) torr.	EX	244-367	(4.10±0.66)(12)	0	138±46	2
OH + CH₃SSCH₃ → products						
Hydroxyl + Disulfide, dimethyl-						
80 COX/SHE ¹⁾ k_{ref} : OH + CH ₂ =CH ₂ → products.	RL	297	(2.8±1.0)(1)			2/2
80 COX/SHE ¹⁾	RN	297	(1.34±0.48)(14)			2
¹⁾ Photolysis of HONO and CH ₃ SSCH ₃ . P = 760 torr.						
81 WIN/KRE Flash-photolysis of H ₂ O/Ar/CH ₃ SSCH ₃ mixtures. P(Ar) = (50-200) torr. P(H ₂ O) = 0.06 torr.	EX	244-367	(3.55±1.99)(13)	0	-380±160	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
<p>OH + NCCN → [C₂N₂OH][†] (a) → HOCN + CN (b)</p>						
<p>Hydroxyl + Ethanedinitrile</p>						
79 PHI1	EX	300-550	(1.87±0.28)(11)	0	1448	2
<p>k_a. Discharge-flow. Resonance-fluorescence. P = (1-16) torr.</p>						
78 ATK/PER2 ¹⁾	EX	298	≤1.81(10)			2
78 ATK/PER2 ¹⁾	EX	424	≤3.01(10)			2
<p>¹⁾ k_b. Flash-photolysis. Resonance-fluorescence. Upper-limit k's.</p>						
<p>OH + CH₃CN → products</p>						
<p>Hydroxyl + Acetonitrile</p>						
81 HAR/KLE	EX	298-424	3.53(11)	0	755±126	2
<p>OH produced by pulsed vacuum-UV photolysis of H₂O in a reaction vessel. Resonance-fluorescence.</p>						
<p>OH + CH₃N=NCH₃ → products</p>						
<p>Hydroxyl + Diazene, dimethyl- (Azomethane)</p>						
79 KLA/AND	EX	368	(4.94±1.33)(11)			2
<p>Flash-photolysis. Resonance-fluorescence.</p>						
<p>OH + CH₃CH₂NH₂ → products</p>						
<p>Hydroxyl + Ethanamine</p>						
78 ATK/PER3	EX	298-426	8.85(12)	0	-189±151	2
<p>Flash-photolysis. Resonance-fluorescence.</p>						
<p>OH + (CH₃)₂NH → H₂O + (CH₃)₂N (a) → H₂O + CH₂NHCH₃ (b)</p>						
<p>Hydroxyl + Methanamine, N-methyl-</p>						
79 LIN/CAL	RL	298	(3.7±0.5)(-1)			2/2
<p>k_a/(k_a + k_b). Long-path FTIR-Spectroscopy.</p>						
78 ATK/PER3	EX	298-426	1.7(13)	0	-247±150	2
<p>k_a + k_b. Flash-photolysis. Resonance-fluorescence.</p>						
<p>OH + CH₃C(O)O₂NO₂ → products</p>						
<p>Hydroxyl + Peroxide, acetyl nitro-</p>						
77 WIN/LLO	EX	299	≤1.0(11)			2
<p>Upper-limit k.</p>						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₃CH₂ONO → products						
Hydroxyl + Nitrous acid ethyl ester (Ethyl nitrite)						
82 AUD/BAU1	EX	295	(1.15±0.23)(12)			2
Static system. OH generated by the reaction:						
$H_2O_2 + NO_2 + CO.$						
P < 75 torr. [CO] ₀ ~ 3.0x10 ¹⁸ molec.cm ⁻³ .						
[CH ₃ CH ₂ ONO] ₀ < 3.6x10 ¹⁷ molec.cm ⁻³ .						
[H ₂ O ₂] ₀ ~ 9.0x10 ¹⁵ molec.cm ⁻³ .						
[NO ₂] ₀ ~ 3.3x10 ¹⁶ molec.cm ⁻³ .						
OH + O=C=C=O → CO₂ + CH=C=O						
Hydroxyl + 1,2-Propadiene-1,3-dione						
77 FAU/WAG2	EX	295-480	(7.0±3.0)(12)	0	620±160	2
OH + CH₃C≡CH → products						
Hydroxyl + 1-Propyne						
73 BRA/HAC	EX	298	(5.7±1.0)(11)			2
OH + CH₂=C=CH₂ → products						
Hydroxyl + 1,2-Propadiene						
73 BRA/HAC	EX	298	(2.7±1.5)(12)			2
77 ATK/PER3	EX	299-424	3.37(12)	0	-154±151	2
77 ATK/PER3	EX	299	(5.60±0.56)(12)			2
OH + CH₃CH=CH₂ → [CH₃CH=CH₂.OH] → products (a)						
→ H ₂ O + CH ₂ CH=CH ₂ (b)						
→ H + CH ₃ CH ₂ CHO (c)						
→ HCHO + CH ₃ CH ₂ (d)						
→ H + (CH ₃) ₂ CO (e)						
→ CH ₃ CHO + CH ₃ (f)						
Hydroxyl + 1-Propene						
71 MOR/NIK2	RL	300	1.0			2/2
k _a /k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.						
73 SIM/HEI2	RL	373-473	1.93(1)	0	-503	2/2
k _a /k _{ref} . k _{ref} : OH + CO → H + CO ₂ . Rate-ratio expression based on only two values: 75.0 at 373 K and 55.0 at 473 K. The ratio of A-factors, 19.3, is correction for an apparent misprint.						
74 GOR/VOL	RL	298	8.93(1)			2/2
k _a /k _{ref} . k _{ref} : OH + CO → CO ₂ + H.						
76 LLO/DAR2	RL	305	9.7			2/2
k _a /k _{ref} . k _{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₂ → products.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 WIN/LLO k_a/k_{ref} . k_{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	4.9(-1)			2/2
76 WU/JAP k_a/k_{ref} . Cylindrical Pyrex Reactor. k_{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	4.0(-1)			2/2
71 MOR/STE ¹⁾	EX	300	1.02(13)			2 1.25
73 SIM/HEI2 ¹⁾	RN	373-473	8.19(12)	0	50	2
73 SIM/HEI2 ¹⁾ Extrapolated k.	ES	298	6.63(12)			2
73 STU1 ¹⁾	EX	298	(8.73±1.33)(12)			2
74 GOR/VOL ¹⁾	RN	298	(8.07±2.05)(12)			2
75 ATK/PIT ¹⁾	EX	297-425	2.47(12)	0	-544±151	2
75 ATK/PIT ¹⁾	EX	298	(1.5±0.15)(13)			2
75 COX ¹⁾ Expressed as αk with $\alpha \sim 2.4$	RN	300	(2.17±0.24)(13)			2
75 GOR/MUL1 ¹⁾ In an atmosphere of water vapor.	EX	381	(8.6±0.4)(12)			2
75 GOR/MUL1 ¹⁾ In an atmosphere of water vapor.	EX	416	(1.2±0.06)(13)			2
75 PAS/CAR ¹⁾ Expressed as nk (n = stoichiometric factor.)	EX	300	(3.01±0.60)(12)			2
76 LLO/DAR2 ¹⁾	RN	305	(1.75±0.35)(13)			2
76 WIN/LLO ¹⁾ ¹⁾ k_a .	RN	305	(1.49±3.0)			2
78 NIP/PAR k_a . Flash-photolysis. Resonance-absorption.	EX	298	(1.47±0.08)(13)			2
74 STU1 k_a . Pulsed vacuum UV Photolysis. Resonance-fluorescence.	EX	298	(8.73±1.32)(12)			2
77 DAV ²⁾ k_a . M = He. P(He) = 20 torr.	EX	298	(1.54±0.07)(13)			2
77 DAV ²⁾ k_a . M = He. P(He) = 200 torr.	EX	298	(1.58±0.07)(13)			2
²⁾ Flash-photolysis. Resonance-fluorescence.						
78 OVE/PAR2 k_a . M = He, or SF ₆ . P-independent k. Vacuum-UV Photolysis of H ₂ O.	EX	298	(2.5±0.5)(13)			2
78 PIT/ATK k_a . Irradiation of Propene-air mixtures in an all-glass chamber. P(Total) = 760 torr.	RN	298	(1.75±0.36)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A units	k err. factor
78 PIT/ATK k _a . Flash-photolysis. Resonance-fluorescence. P ~ (15-650) torr.	EX	298	(1.51±0.15)(13)			2	
78 RAV/WAG ³) k _a . M = He. P(He) = 20 torr.	EX	298	(1.54±0.07)(13)			2	
78 RAV/WAG ³) k _a . M = He. P(He) = 200 torr. ³) Flash-photolysis. Resonance-fluorescence.	EX	298	(1.58±0.07)(13)			2	
79 NIP/PAR k _a . Flash-photolysis. Resonance-fluorescence.	EX	297	(1.48±0.17)(13)			2	
82 ATK/ASC2 k _a . Mean of three previously reported k's.	SE	299	1.52(13)			2	
73 BRA/HAC k _b .	EX	298	(3.0±1.0)(12)			2	
73 GOR k _b . Lower-limit k.	EX	298	≥8.25(12)			2	
80 COX/DER1 k _b . Photolysis of HONO + CH ₃ CH=CH ₂ at 760 torr. Gas-chromatography. Same data given in 80 COX.	RN	298	1.45(13)			2	
82 BIE/HAR k _b /k _a .	RL	298	<2.0(-2)			2/2	
79 HOY/SIE2 k _d /k _c . Low pressure nozzle reactor. Mass- spectrometry. P ~ (0.2-1.8) torr.	RL	298	(4.0±1.5)			2/2	
79 HOY/SIE2 k _f /k _e . Low pressure nozzle. P ~ (0.2-1.8) torr.	RL	298	(3.5±1.5)			2/2	
OH + CD₃CH=CH₂ → products							
Hydroxyl + 1-Propene-3,3,3-d ₃							
73 STU1	EX	298	(8.73±1.33)(12)			2	
OH + CH₃CD=CD₂ → products							
Hydroxyl + 1-Propene-1,1,2-d ₃							
73 STU1	EX	298	(8.73±1.33)(12)			2	
OH + CD₃CD=CD₂ → products							
Hydroxyl + 1-Propene-d ₆							
71 MOR/NIK2	RL	300	1.1			2/2	
k _{ref} : OH + CH ₃ CH=CH ₂ → products.							
73 STU1	EX	298	(1.01±0.15)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH ₃ CH ₂ CH ₃ → H ₂ O + (CH ₃) ₂ CH (a) → H ₂ O + CH ₃ CH ₂ CH ₂ (b)						
Hydroxyl + Propane						
71 BAK/BAL k _a . Rate constant per secondary CH bond.	CO	298-753	2.2(13)	0	1283	2
71 BAK/BAL ¹⁾ k _a /k _{ref} . Estimated ratio per primary CH bond.	RL	753	5.25			2/2
78 DAR/ATK k _a . Irradiation technique. k computed from an empirical formula.	CO	300	6.99(11)			2
79 BAL/WAL1 ¹⁾ k _a /k _{ref} . A and B recalculated from an empirical formula.	RL	753-773	3.46(-1)	0	-1820	2/2
82 ATK/ASC3 k _a . Calculated from an empirical formula.	RN	299	5.06(11)			2
71 BAK/BAL ¹⁾ k _b /k _{ref} . Estimated ratio per secondary CH bond.	RL	753	1.1(1)			2/2
78 DAR/ATK k _b . Irradiation technique. k computed from an empirical formula.	CO	300	2.35(11)			2
79 BAL/WAL1 ¹⁾ k _b /k _{ref} . Calculated from an empirical formula.	RL	753-773	1.28	0	-1070	2/2
¹⁾ k _{ref} : OH + H ₂ → H ₂ O + H.						
82 ATK/ASC3 k _b .	ES	299	1.14(11)			2
73 BRA/HAC ²⁾	EX	298	(5.0±1.0)(11)			2
73 GOR ²⁾	EX	298	(1.17±0.18)(12)			2
74 GOR/VOL ²⁾	RN	298	(1.33±0.36)(12)			2
75 GOR/MUL1 ²⁾ In an atmosphere of water vapor.	EX	381	(1.3±0.06)(12)			2
75 GOR/MUL1 ²⁾ In an atmosphere of water vapor.	EX	416	(1.15±0.05)(12)			2
75 HAR/BUR ²⁾	EX	329	(1.19±0.05)(12)			2
75 OVE/PAR ²⁾	EX	295	(1.22±0.06)(12)			2
78 DAR/ATK ²⁾ Irradiation technique.	EX	300	(9.58±1.33)(11)			2
80 COX/DER1 ²⁾ HONO photosensitized oxidation in synthetic air. [HONO] = (3-20) ppm. [NO] = NO ₂] = (0.3-3.0) Same data given in 80 COX.	RN	300	1.14(12)			2
²⁾ k _a + k _b .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC3 ³) $k_a + k_b$.	RN	299	(7.35±0.30)(11)			2
71 BAK/BAL ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H.	RL	753	(2.15±0.22)(1)			2/2
74 GOR/VOL ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CO → CO ₂ + H.	RL	298	1.43(1)			2/2
75 HUC/BOO ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CH ₃ CH ₃ → H ₂ O + CH ₃ CH ₂	RL	653	(2.18±0.28)			2/2
82 ATK/ASC3 ³) ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	299	(4.73±0.16)(-1)			2
3) Photolysis of CH ₃ ONO/NO/Propane mixtures. P(Total) = 735 torr. [NO] ₀ = 1.2x10 ¹⁴ molec.cm ⁻³ . [Propane] = (1.2-2.4)x10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (2.1-4.0)x10 ¹⁴ molec.cm ⁻³ .						
OH + CH ₂ =CHCHO → H ₂ O + CH ₂ =CHCO (a) → any other products (b)						
Hydroxyl + 2-Propenal (Acrolein)						
80 MAL/CHI k_a . Photooxidation of 2-Propenal/Butane/Nitric oxide/Air mixtures in a smog chamber. k determined relative to the reaction: OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RN	298	(1.6±0.2)(13)			2
81 KER/SHE ¹) $k_{overall}/k_{ref}$. k_{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(2.38±0.28)			2/2
81 KER/SHE ¹) $k_{overall}$.	RN	298	(1.14±0.12)(13)			2
1) HONO/Synthetic air/Ethene/aldehyde photolysis.						
OH + CH ₃ C(O)CHO → products						
Hydroxyl + Propanal, 2-oxo- (Methylglyoxal)						
82 KLE/HAR OH generated by H ₂ O photolysis in Ar. Resonance-fluorescence. P(Total) = 50 torr.	EX	297	(4.28±0.96)(12)			2
OH + CH ₂ =CHCH ₂ OH → products						
Hydroxyl + 2-Propen-1-ol (Allyl alcohol)						
75 GOR/MUL1 In an atmosphere of water vapor.	EX	440	(1.56±0.2)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₂=CHOCH₃ → products						
Hydroxyl + Ethene, methoxy-						
77 PER/ATK1	EX	299-427	3.67(12)	0	-511±151	2
77 PER/ATK1	EX	299	(2.02±0.20)(13)			2
OH + CH₃CH₂CHO → H₂O + CH₃CH₂CO (a)						
→ H ₂ O + CH ₃ CHCHO (b)						
→ H ₂ O + CH ₂ CH ₂ CHO (c)						
Hydroxyl + Propanal						
71 MOR/NIK2	RL	300	1.8			2/2
(k _a + k _b + k _c)/k _{ref} .						
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
72 VOL/GOR	EX	298	(2.29±0.90)(12)			2
k _a + k _b + k _c .						
78 NIK/MAK ¹⁾	RL	298	(2.6±0.1)			2
k _{ref} : OH + CH ₂ =CH ₂ → products.						
78 NIK/MAK ¹⁾	RN	298	1.26(13)			2
¹⁾ k _a + k _b + k _c . CH ₃ CH ₂ CHO/HONO Photolysis.						
FTIR-Spectroscopy.						
P(air) = 700 torr.						
81 AUD/BAU ²⁾	RL	298	(1.14±0.13)			2/2
(k _a + k _b + k _c)/k _{ref} .						
k _{ref} : OH + CH ₃ CHO → products.						
81 AUD/BAU ²⁾	RN	298	(1.08±0.14)(13)			2
k _a + k _b + k _c .						
²⁾ Linear, boric-acid-coated flow tube. Gas-chromatography.						
Channel (a) is predominant.						
P(Total) = 299 torr.						
81 KER/SHE ³⁾	RL	298	(2.28±0.17)			2/2
(k _a + k _b + k _c)/k _{ref} .						
k _{ref} : OH + CH ₂ =CH ₂ → products.						
81 KER/SHE ³⁾	RN	298	(1.08±0.06)(13)			2
k _a + k _b + k _c .						
³⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.						
OH + (CH₃)₂CO → H₂O + CH₂C(O)CH₃						
Hydroxyl + 2-Propanone						
80 COX/DER1	RN	300	3.01(11)			2
HONO photosensitized oxidation in synthetic air.						
Gas-chromatography. Same data given in 80 COX.						
[NO] = NO ₂ = (0.3-3.0) ppm.						
[HONO] = (3-20) ppm.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + CH₃CH₂COOH → products							
Hydroxyl + Propanoic acid							
82 ZET/STU	EX	298	(9.64±0.72)(11)				2
H ₂ O/Ar/Propanoic acid photolysis. Resonance-fluorescence.							
P(H ₂ O) = (0.02-0.22) torr.							
P(Ar) = 100 torr.							
OH + CH₃C(O)OCH₃ → H₂O + CH₃C(O)OCH₂ (a) → H₂O + CH₂C(O)OCH₃ (b)							
Hydroxyl + Acetic acid methyl ester (Methyl acetate)							
78 CAM/PAR	EX	292	(1.1±0.3)(11)				2
k _a + k _b . Reaction in a Pyrex vessel. Vacuum system. OH generated by reaction of a H ₂ O ₂ /NO ₂ /CO mixture. Channel (a) preferred.							
P(NO ₂) = 2.1 torr. P(Total) = 100 torr.							
OH + CH₃CH₂CH₂OH → products							
Hydroxyl + 1-Propanol							
76 CAM/MCL	EX	292	(2.3±0.2)(12)				2
78 OVE/PAR1	EX	296	(3.21±0.32)(12)				2
Flash-photolysis. Resonance-absorption.							
OH + (CH₃)₂CHOH → products							
Hydroxyl + 2-Propanol							
76 LLO/DAR1	RL	305	1.4(-1)				2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.							
76 LLO/DAR1	RN	305	(4.3±1.3)(12)				2
78 OVE/PAR1	EX	296	(3.30±0.33)(12)				2
Flash-photolysis. Resonance-absorption.							
OH + CH₂=CHCN → products							
Hydroxyl + 2-Propenenitrile (Acrylonitrile)							
81 HAR/KLE	EX	298-424	(2.43±0.03)(12)	0	0		2
OH produced by UV photolysis of H ₂ O under flow conditions. Resonance-fluorescence.							
OH + CH₃CH₂CN → products							
Hydroxyl + Propanenitrile							
81 HAR/KLE	EX	298-424	1.62(11)	0	800±176		2
OH produced by UV photolysis of H ₂ O under flow conditions. Resonance-fluorescence.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH₃)₃N → products						
Hydroxyl + Methanamine, N,N-dimethyl-						
78 ATK/PER3 Flash-photolysis. Resonance-fluorescence.	EX	298-426	1.58(13)	0	-252±151	2
OH + CH₃CH₂CH₂ONO → products						
Hydroxyl + Nitrous acid propyl ester						
82 AUD/BAU1 Static system. OH generated by the chain reaction:	EX	295	(1.56±0.32)(12)			2
$\text{H}_2\text{O}_2 + \text{NO}_2 + \text{CO}.$ $[\text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}]_0 < 3.6 \times 10^{17} \text{ molec. cm}^{-3}.$ $[\text{H}_2\text{O}_2]_0 \sim 9.0 \times 10^{15} \text{ molec. cm}^{-3}.$ $[\text{NO}_2]_0 \sim 3.3 \times 10^{16} \text{ molec. cm}^{-3}.$ $[\text{CO}]_0 \sim 3.0 \times 10^{18} \text{ molec. cm}^{-3}.$ P < 75 torr.						
OH + (CH₃)₂CHONO₂ → products						
Hydroxyl + Nitric acid 1-methylethyl ester (Isopropyl nitrate)						
82 ATK/ASC5 ¹⁾	RL	299	(2.4±0.6)(-2)			2/2
$k_{\text{ref}}: \text{OH} + \text{C}_6\text{H}_{10} \rightarrow \text{products}.$						
82 ATK/ASC5 ¹⁾	RN	299	(1.08±0.30)(11)			2
¹⁾ Photolysis of CH ₃ ONO/NO/Isopropyl nitrate. $[\text{CH}_3\text{ONO}]_0 = (0.9-7.1) \times 10^{14} \text{ molec. cm}^{-3}.$ $[\text{Alkyl nitrate}] = 2.4 \times 10^{13} \text{ molec. cm}^{-3}.$						
OH + CH=CC=CH → CH=CCH=C=O + H						
Hydroxyl + 1,3-Butadiyne						
82 BIT/HOW C ₆ H ₆ /O ₂ /Ar flame. P = 20 torr.	ES	1700-1900	(5.0±2.0)(12)	0	0	2
OH + CH₂=CHCH=CH₂ → products						
Hydroxyl + 1,3-Butadiene						
76 LLO/DAR2 $k_{\text{ref}}: \text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}.$	RL	305	2.58(1)			2/2
76 LLO/DAR2	RN	305	(4.64±0.93)(13)			2
77 ATK/PER3	EX	299-424	8.73(12)	0	-468±151	2
77 ATK/PER3	EX	299	(4.13±0.42)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + CH ₃ CH ₂ CH=CH ₂ → H ₂ O + CH ₃ CHCH=CH ₂ (a)							
→ CH ₃ CH ₂ CH(OH)CH ₂ (b)							
→ CH ₃ CH ₂ CHCH ₂ OH (c)							
→ any other products (d)							
Hydroxyl + 1-Butene							
82 BIE/HAR ¹)	RL	298	(2.0±0.6)(-1)				2/2
k _a /(k _a + k _b + k _c).							
82 BIE/HAR ¹)	EX	298	(1.81±0.24)(13)				2
k _a + k _b + k _c .							
¹) Discharge-flow. OH generated by reacting H with NO ₂ . [OH] ₀ = (0.2-2.0) × 10 ¹² molec. cm ⁻³ . P(Total) ~ 2 torr.							
71 MOR/NIK2	RL	300	2.4				2/2
k _{overall} . k _{ref} : OH + CH ₃ CH=CH ₂ → products.							
75 ATK/PIT ²)	EX	297-425	4.58(12)	0	-468±151		2
75 ATK/PIT ²)	EX	298	(2.13±0.22)(13)				2
²) k _{overall} .							
75 PAS/CAR	EX	300	(9.03±0.60)(12)				2
k _{overall} . Expressed as nk.							
(n = stoichiometric factor.)							
76 WU/JAP	RL	303	5.2(-1)				2/2
k _{overall} . Cylindrical Pyrex Reactor.							
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.							
P = 760 torr.							
77 DAV ³)	EX	298	(1.78±0.11)(13)				2
k _{overall} . M = He. P(He) = 3 torr.							
77 DAV ³)	EX	298	(1.77±0.08)(13)				2
k _{overall} . M = He. P(He) = 200 torr.							
78 PIT/ATK ³)	EX	298	(2.13±0.22)(13)				2
k _{overall} . P ~ (15-650) torr.							
78 RAV/WAG ³)	EX	298	(1.78±0.11)(13)				2
k _{overall} . M = He. P(He) = 3 torr.							
78 RAV/WAG ³)	EX	298	(1.77±0.08)(13)				2
k _{overall} . M = He. P(He) = 20 torr.							
79 NIP/PAR ³)	EX	297	(2.01±0.15)(13)				2
k _{overall} .							
³) Flash-photolysis. Resonance-fluorescence.							
OH + cis-CH ₃ CH=CHCH ₃ → products							
Hydroxyl + 2-Butene, (Z)-							
71 MOR/NIK2	RL	300	3.6				2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.							


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 ATK/PIT	EX	297-425	6.26(12)	0	-488±151	2
75 ATK/PIT	EX	298	(3.23±0.32)(13)			2
76 LLO/DAR2	RL	305	2.18(1)			2/2
k _{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.						
76 LLO/DAR2	RN	305	(3.92±0.80)(13)			2
76 WIN/LLO	RL	305	1.22			2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 WIN/LLO	RN	305	(3.72±0.56)(13)			2
77 DAV ¹)	EX	298	(2.60±0.24)(13)			2
M = He. P(He) = 3 torr.						
77 DAV ¹)	EX	298	(2.57±0.15)(13)			2
M = He. P(He) = 20 torr.						
¹) Flash-photolysis. Resonance-fluorescence.						
78 PIT/ATK	RN	298	(3.91±0.78)(13)			2
Propene/Air irradiation.						
P(Total) = 1 atm.						
78 PIT/ATK	EX	298	(3.23±0.33)(13)			2
Flash-photolysis. Resonance-fluorescence.						
P ~ (15-650) torr.						
78 RAV/WAG ²)	EX	298	(2.60±0.24)(13)			2
M = He. P(He) = 3 torr.						
78 RAV/WAG ²)	EX	298	(2.57±0.15)(13)			2
M = He. P(He) = 20 torr.						
²) Flash-photolysis. Resonance-fluorescence.						
OH + trans-CH₃CH=CHCH₃ → products						
Hydroxyl + 2-Butene, (E)-						
71 MOR/NIK2	RL	300	4.2			2/2
k _{ref} : OH + CH ₃ CH ₃ CH ₂ → products.						
75 ATK/PIT	EX	297-425	6.74(12)	0	-549±151	2
75 ATK/PIT	EX	298	(4.21±0.42)(13)			2
75 COX	RN	300	(6.38±1.63)(13)			2
k expressed as αk						
with α ~ 1.7						
75 PAS/CAR	EX	300	(7.23±6.02)(12)			2
k expressed as nk.						
(n = stoichiometric factor.)						
76 WU/JAP	RL	303	1.3			2/2
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.						
P = 760 torr.						
78 PIT/ATK	EX	298	(4.21±0.42)(13)			2
Propene/air irradiation.						
P(Total) = 760 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
OH + (CH ₃) ₂ C=CH ₂ → H ₂ O + CH ₂ =C(CH ₃)CH ₂ (a) → (CH ₃) ₂ C(OH)CH ₂ (b) → (CH ₃) ₂ CCH ₂ OH (c)							
Hydroxyl + 1-Propene, 2-methyl-							
78 BAK/BAL ¹) k _a . Possibly an upper-limit.	ES	753	2.9(13)			2	
78 BAK/BAL ¹) (k _b + k _c)/k _a .	RL	753	3.7			2/2	
78 BAK/BAL ¹) k _b + k _c .	ES	753	7.8(12)			2	2.0
¹) Oxidation in aged boric-acid-coated vessels. P(Total) = (490-505) torr.							
71 MOR/NIK2 k _{overall} /k _{ref} . k _{ref} : OH + CH ₃ CH=CH ₂ → products.	RL	300	3.8			2/2	
75 ATK/PIT ²)	EX	297-425	5.54(12)	0	-503±151	2	
75 ATK/PIT ²) ²) k _{overall} .	EX	298	(3.05±0.31)(13)			2	
76 WU/JAP k _{overall} /k _{ref} . P = 760 torr. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.	RL	303	9.2(-1)			2/2	
78 PIT/ATK k _{overall} . Flash-photolysis. Resonance-fluorescence. P ~ (15-650) torr.	EX	298	(3.05±0.31)(13)			2	
OH + □ → H ₂ O + □*							
Hydroxyl + Cyclobutane							
74 GOR/VOL ¹)	RL	298	8.47			2/2	
74 GOR/VOL ¹) ¹) Uncorrected for n-Butane impurity.	RN	298	7.83(11)			2	
74 GOR/VOL Corrected for n-Butane impurity.	RN	298	(7.23±1.81)(11)			2	
OH + CH ₃ CH ₂ CH ₂ CH ₃ → H ₂ O + CH ₃ CH ₂ CH ₂ CH ₂ (a) → H ₂ O + CH ₃ CH ₂ CHCH ₃ (b)							
Hydroxyl + Butane							
71 BAK/BAL k _a /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio per primary CH bond.	RL	753	5.25			2/2	
79 BAL/WAL1 k _a /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. A and B recalculated from a given empirical formula.	RL	753-773	1.28	0	-1070	2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 BAK/BAL k_b/k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio per secondary CH bond.	RL	753	1.175(1)			2/2
79 BAL/WAL1 k_b/k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H. A and B recalculated from given empirical formula.	RL	753-773	6.92(-1)	0	-1820	2/2
71 BAK/BAL ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H.	RL	753	(3.40±0.34)(1)			2/2
71 MOR/NIK2 ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CH ₃ CH=CH ₂ → products.	RL	300	2.4(-1)			2/2
74 GOR/VOL ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CO → H + CO ₂ .	RL	298	1.94(1)			2/2
75 CAM/HAN1 ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CO → H + CO ₂	RL	292	(1.48±0.09)(1)			2/2
75 HUC/BOO ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CH ₃ CH ₂ CH ₃ → H ₂ O + CH ₃ CH ₂ CH ₂ (C) → H ₂ O + (CH ₃) ₂ CH (d)	RL	653	(1.54±0.13)			2/2
82 ATK/ASC2 1) ($k_a + k_b$)/ k_{ref} . k_{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(4.53±0.07)(-1)			2/2
82 ATK/ASC2 1) ($k_a + k_b$)/ k_{ref} . k_{ref} : OH +  → products.	RL	299	(3.41±0.02)(-1)			2/2
73 GOR 2)	EX	298	(1.97±0.05)(12)			2
73 STU2 2)	EX	298	(1.42±0.21)(12)			2
74 GOR/VOL 2)	RN	298	(1.75±0.42)(12)			2
75 GOR/MUL1 2) M = Ar (710 torr.) + H ₂ O (10 torr.) + C ₄ H ₁₀ (0.54-2.46 torr.)	EX	298	(2.54±0.1)(12)			2
75 GOR/MUL1 2) P = (0.5-198) torr. In an atmosphere of water vapor.	EX	381	(2.5±0.1)(12)			2
75 GOR/MUL1 2) P = (0.5-198) torr. In an atmosphere of water vapor.	EX	416	(3.0±0.1)(12)			2
76 PER/ATK2 2)	EX	297-420	1.06(13)	0	559±151	2
76 PER/ATK2 2)	EX	297	(1.64±0.16)(12)			2
80 PAR/NIP 2) Flash-photolysis. Resonance-absorption.	EX	297	(1.61±0.13)(12)			2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC2 ¹⁾ 2) Mean of four previously reported k's.	SE	299	1.55(12)			2
1) CH ₃ ONO/NO/CH ₃ CH ₂ CH ₂ CH ₃ /Cyclohexane (or Hexane) photolysis. [CH ₃ ONO] ₀ = (9.5-3.5)x10 ¹⁴ molec.cm ⁻³ . [Butane] ₀ = (1.2-2.4)x10 ¹³ molec.cm ⁻³ . P(Total) = 735 torr.						
82 AUD/BAU1 ²⁾ Static system. OH generated by the chain reaction: H ₂ O ₂ + NO ₂ + CO. P < 75 torr. [CO] ₀ ~ 3.0x10 ¹⁸ molec.cm ⁻³ . [Butane] ₀ < 3.6x10 ¹⁷ molec.cm ⁻³ . [H ₂ O ₂] ₀ ~ 9.0x10 ¹⁵ molec.cm ⁻³ . [NO ₂] ₀ ~ 3.3x10 ¹⁶ molec.cm ⁻³ .	EX	295	(1.63±0.16)(12)			2
2) k _a + k _b .						
OH + CD ₃ CD ₂ CD ₂ CD ₃ → HDO + CD ₃ CD ₂ CD ₂ CD ₂ (a) → HDO + CD ₃ CD ₂ CD ₂ CD ₃ (b)						
Hydroxyl + Butane-d ₁₀						
80 PAR/NIP k _a + k _b . Flash-photolysis. Resonance-absorption.	EX	297	(4.20±0.41)(11)			2
OH + CH ₃ CH ₂ CH ₂ CH ₃ → HDO + CH ₃ CH ₂ CH ₂ CH ₂ (a) → HDO + CH ₃ CH ₂ CH ₂ CH ₃ (b)						
Hydroxyl-d + Butane						
80 PAR/NIP k _a + k _b . Flash-photolysis. Resonance-absorption.	EX	297	(1.66±0.13)(12)			2
OH + CD ₃ CD ₂ CD ₂ CD ₃ → D ₂ O + CD ₃ CD ₂ CD ₂ CD ₂ (a) → D ₂ O + CD ₃ CD ₂ CD ₂ CD ₃ (b)						
Hydroxyl-d + Butene-d ₁₀						
80 PAR/NIP k _a + k _b . Flash-photolysis. Resonance-absorption.	EX	297	(4.84±0.38)(11)			2
OH + (CH ₃) ₃ CH → H ₂ O + (CH ₃) ₃ C (a) → H ₂ O + (CH ₃) ₂ CHCH ₂ (b)						
Hydroxyl + Propane, 2-methyl-						
71 BAK/BAL k _a . Rate constant per tertiary CH bond.	CO	298-753	5.3(13)	0	1203	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 BAK/BAL k_a/k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio per tertiary CH bond.	RL	753	1.525(1)			2/2
72 GOR/VOL k_a/k_{ref} . k_{ref} : OH + CO → H + CO ₂	RL	298	(2.33±0.07)(1)			2/2
72 GOR/VOL k_a . Similar data in 72 VOL/GOR and 73 GOR.	RN	298	(2.11±0.48)(12)			2
78 DAR/ATK k_a . Irradiation technique. Computed from an empirical formula.	CO	300	1.26(12)			2
79 BAL/WAL1 ¹⁾ k_a/k_{ref} . A and B recalculated from a given empirical formula. k_{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	2.73(-1)	0	-2060	2/2
81 BAL/WAL2 ¹⁾ k_a . ¹⁾ Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures in aged boric-acid-coated vessels. Gas-chromatography. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.	ES	300-1500	2.57(12)	0	271±96	2 1.2
71 BAK/BAL k_b/k_{ref} . k_{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio per primary CH bond.	RL	753	5.25			2/2
78 DAR/ATK k_b . Irradiation technique. Computed from an empirical formula.	CO	300	3.5(11)			2
79 BAL/WAL1 k_b/k_{ref} . A and B recalculated from an empirical formula. k_{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	1.93	0	-1070	2/2
71 BAK/BAL $(k_a + k_b)/k_{ref}$. k_{ref} : OH + H ₂ → H ₂ O + H.	RL	753	(3.10±0.31)(1)			2/2
75 HUC/BOO $(k_a + k_b)/k_{ref}$. k_{ref} : OH + CH ₃ CH ₂ CH ₃ → H ₂ O + (CH ₃) ₂ CH (c) → H ₂ O + CH ₃ CH ₂ CH ₂ (d)	RL	653	(1.28±0.07)			2/2
76 WU/JAP $(k_a + k_b)/k_{ref}$. Pyrex Reactor. P = 760 torr. k_{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.	RL	303	4.0(-2)			2/2
78 BUT/SOL $k_a + k_b$. Quartz reactor. H ₂ O ₂ photolysis. Gas-chromatography. P(O ₂ + N ₂) >100 torr.	RN	305	(9.58±1.08)(11)			2
78 DAR/ATK $k_a + k_b$. Irradiation technique.	EX	300	(1.53±0.03)(12)			2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH +  → products						
Hydroxyl + Furan						
82 LEE/TAN Discharge-flow. Resonance-fluorescence. OH generated by reacting H with NO ₂ .	EX	295	(6.32±0.48)(13)			2
OH + CH ₃ CH=CHCHO → products						
Hydroxyl + 2-Butenal (Crotonaldehyde)						
81 KER/SHE ¹⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(4.12±0.80)			2/2
81 KER/SHE ¹⁾ ¹⁾ Photolysis of HONO/Synthetic air mixtures containing low concentrations of Ethene and aldehyde.	RN	298	(1.99±0.36)(13)			2
OH + CH ₃ C(O)CH=CH ₂ → products						
Hydroxyl + 3-Buten-2-one						
80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas-chromatography. Same data given in 80 COX. [NO] = [NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm.	RN	300	8.43(12)			2
82 KLE/HAR M = Ar. OH generated by photolysis of water vapor. Flash-photolysis. Resonance-fluorescence. P(Total) = 50 torr.	EX	297-424	2.32(12)	0	-456±73	2
OH + CH ₂ =C(CH ₃)CHO → products						
Hydroxyl + 2-Propenal, 2-methyl- (Methacrolein)						
82 KLE/HAR M = Ar. OH generated by Photolysis of Water vapor. Flash-photolysis. Resonance-fluorescence. P(Total) = 50 torr.	EX	297-424	1.07(13)	0	-175±52	2
OH + CH ₃ CH ₂ CH ₂ CHO → H ₂ O + CH ₃ CH ₂ CH ₂ CO (a) → H ₂ O + CH ₃ CH ₂ CHCHO (b) → H ₂ O + CH ₃ CHCH ₂ CHO (c) → H ₂ O + CH ₂ CH ₂ CH ₂ CHO (d)						
Hydroxyl + Butanal						
81 AUD/BAU ¹⁾ (k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₃ CHO → products.	RL	298	(1.62±0.20)			2/2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 AUD/BAU ¹⁾ $k_a + k_b + k_c + k_d$.	RN	298	(1.52±0.19)(13)			2
¹⁾ Linear, boric-acid-coated flow tube. Gas-chromatography. Channel (a) is predominant. P(Total) = 299 torr.						
81 KER/SHE ²⁾ $k_{ref}: OH + CH_2=CH_2 \rightarrow \text{products}$.	RL	298	(2.96±0.07)			2/2
81 KER/SHE ²⁾ ²⁾ Photolysis of HONO/Synthetic air mixtures containing low concentrations of Ethene and aldehyde.	EX	298	(1.45±0.06)(13)			2
$OH + (CH_3)_2CHCHO \rightarrow H_2O + (CH_3)_2CHCO$ (a) $\rightarrow H_2O + (CH_3)_2CHCHO$ (b) $\rightarrow H_2O + CH_2CH(CH_3)CHCHO$ (c)						
Hydroxyl + Propanal, 2-methyl-						
79 BAL/CLE k_b/k_a . Oxidation in an aged boric-acid-coated vessel. P(Total) = 60 torr.	RL	713	(7.0±1.0)(-1)			2
81 AUD/BAU ¹⁾ $(k_a + k_b + k_c)/k_{ref}$. $k_{ref}: OH + CH_3CHO \rightarrow \text{products}$.	RL	298	(1.12±0.13)			2/2
81 AUD/BAU ¹⁾ $k_a + k_b + k_c$.	RN	298	(1.05±0.12)(13)			2
¹⁾ Linear, boric-acid-coated flow tube. Gas-chromatography. Channel (a) is predominant. P(Total) = 299 torr.						
81 KER/SHE ²⁾ $(k_a + k_b + k_c)/k_{ref}$. $k_{ref}: OH + CH_2=CH_2 \rightarrow \text{products}$.	RL	298	(3.40±0.66)			2/2
81 KER/SHE ²⁾ $k_a + k_b + k_c$.	RN	298	(1.63±0.06)(13)			2
²⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.						
OH + $CH_3C(O)CH_2CH_3 \rightarrow \text{products}$						
Hydroxyl + 2-Butanone						
76 WIN/LLO $k_{ref}: OH + (CH_3)_2C=CH_2 \rightarrow \text{products}$.	RL	305	7.0(-2)			2/2
76 WIN/LLO	RN	305	(2.0±0.6)(12)			2
80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas chromatography. Same data given in 80 COX. [NO] = NO ₂ = (0.3-3.0) ppm. [HONO] = (3-20) ppm.	RN	300	1.57(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 COX/PAT ¹⁾ k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	296	(0.11±0.01)			2/2
81 COX/PAT ¹⁾ ¹⁾ Photolysis of HONO diluted N ₂ /O ₂ mixtures, in presence of Butane. P = 760 torr.	RN	296	(5.30±0.54)(11)			2
OH + CH₃CH₂CH₂COOH → products						
Hydroxyl + Butanoic acid						
82 ZET/STU Pulsed vacuum UV-Photolysis of H ₂ O, Ar and Butanoic acid mixtures. Resonance-fluorescence. P(Ar) = (30-300) torr. P(H ₂ O) = (0.04-0.1) torr.	EX	298	(1.08±0.10)(12)			2
OH + CH₃C(O)OCH₂CH₃ → products						
Hydroxyl + Acetic acid ethyl ester (Ethyl acetate)						
78 CAM/PAR Reaction of ester vapor with OH. Vacuum system. OH generated by reaction of a H ₂ O ₂ /NO ₂ /CO mixture. P(Total) = 100 torr. P(NO ₂) = 2.1 torr.	EX	292	(1.16±0.13)(12)			2
OH + CH₃CH₂C(O)OCH₃ → products						
Hydroxyl + Propanoic acid methyl ester						
78 CAM/PAR Reaction of ester vapor with OH. Vacuum system. OH generated by reaction of a H ₂ O ₂ /NO ₂ /CO mixture. P(Total) = 100 torr. P(NO ₂) = 2.1 torr.	EX	292	(1.7±0.6)(11)			2
OH +  → products						
Hydroxyl + Furan, tetrahydro-						
77 WIN/LLO k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	2.9(-1)			2/2
77 WIN/LLO	RN	305	(8.8±1.8)(12)			2
78 RAV/DAV ¹⁾ M = He. P(He) = 20 torr.	EX	298	(9.82±0.96)(12)			2
78 RAV/DAV ¹⁾ M = He. P(He) = 200 torr.	EX	298	(9.58±2.35)(12)			2
¹⁾ Flash-photolysis. Resonance-fluorescence.						
OH + CH₃CH₂CH₂CH₂OH → products						
Hydroxyl + 1-Butanol						
76 CAM/MCL	EX	292	(4.1±0.6)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH₃CH₂)₂O → products						
Hydroxyl + Ethane, 1,1'-oxybis-						
76 LLO/DAR1	RL	305	1.85(-1)			2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 LLO/DAR1	RN	305	(5.6±1.1)(12)			2
OH + (CH₃)₃COOH → products						
Hydroxyl + Hydroperoxide, 1,1-dimethylethyl-						
78 ANA/SMI2	EX	298	(1.81±0.48)(12)			2
Flash-photolysis of (CH ₃) ₃ COOH/H ₂ O mixtures.						
[(CH ₃) ₃ COOH] = (0.8-2.0) × 10 ¹⁵ molec. cm ³ .						
[H ₂ O] = ~1.5 × 10 ¹⁶ molec. cm ³ .						
OH +  → products						
Hydroxyl + Thiophene						
82 LEE/TAN	EX	295	(2.87±0.38)(13)			2
Discharge-flow. Resonance-fluorescence.						
OH generated by reacting H with NO ₂ .						
OH + CH₃CH₂CH₂CH₂ONO → products						
Hydroxyl + Nitrous acid butyl ester (n-Butyl nitrite)						
82 AUD/BAU1	EX	295	(3.41±1.48)(12)			2
Static system. OH generated by the chain reaction:						
H ₂ O ₂ + NO ₂ + CO.						
P < 75 torr. [CO] ₀ ~ 3.0 × 10 ¹⁸ molec. cm ⁻³ .						
[CH ₃ (CH ₂) ₃ ONO] ₀ < 3.6 × 10 ¹⁷ molec. cm ⁻³ .						
[H ₂ O ₂] ₀ ~ 9.0 × 10 ¹⁵ molec. cm ⁻³ .						
[NO ₂] ₀ ~ 3.3 × 10 ¹⁶ molec. cm ⁻³ .						
OH + CH₃CH₂CH(CH₃)ONO → products						
Hydroxyl + Nitrous acid 1-methylpropyl ester (s-Butyl nitrite)						
82 AUD/BAU1	EX	295	(3.89±0.58)(12)			2
Static system. OH generated by the chain reaction:						
H ₂ O ₂ + NO ₂ + CO.						
[CH ₃ CH ₂ CH(CH ₃)ONO] ₀ < 3.6 × 10 ¹⁷ molec. cm ⁻³ .						
P < 75 torr. [CO] ₀ ~ 3.0 × 10 ¹⁸ molec. cm ⁻³ .						
[H ₂ O ₂] ₀ ~ 9.0 × 10 ¹⁵ molec. cm ⁻³ .						
[NO ₂] ₀ ~ 3.3 × 10 ¹⁶ molec. cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH₃)₂CHCH₂ONO → products						
Hydroxyl + Nitrous acid 2-methylpropyl ester (iso-Butyl nitrite)						
82 AUD/BAU1	EX	295	(3.47±0.52)(12)			2
Static system. OH generated by the chain reaction: $H_2O_2 + NO_2 + CO.$ $P < 75 \text{ torr. } [CO]_0 \sim 3.0 \times 10^{18} \text{ molec.cm}^{-3}.$ $[(CH_3)_2CHCH_2ONO]_0 < 3.6 \times 10^{17} \text{ molec.cm}^{-3}.$ $[H_2O_2]_0 \sim 9.0 \times 10^{15} \text{ molec.cm}^{-3}.$ $[NO_2]_0 \sim 3.3 \times 10^{16} \text{ molec.cm}^{-3}.$						
OH + (CH₃)₃CONO → products						
Hydroxyl + Nitrous acid 1,1-dimethylethyl ester (t-Butyl nitrite)						
82 AUD/BAU1	EX	295	(9.1±1.5)(11)			2
Static system. OH generated by the chain reaction: $H_2O_2 + NO_2 + CO.$ $P < 75 \text{ torr. } [CO]_0 \sim 3.0 \times 10^{18} \text{ molec.cm}^{-3}.$ $[(CH_3)_3CONO]_0 < 3.6 \times 10^{17} \text{ molec.cm}^{-3}.$ $[H_2O_2]_0 \sim 9.0 \times 10^{15} \text{ molec.cm}^{-3}.$ $[NO_2]_0 \sim 3.3 \times 10^{16} \text{ molec.cm}^{-3}.$						
OH + CH₃CH₂CH₂CH₂ONO₂ → products						
Hydroxyl + Nitric acid butyl ester (n-Butyl nitrate)						
82 ATK/ASC5 ¹⁾	RL	299	(1.87±0.14)(-1)			2/2 ₄
$k_{ref}: OH + \text{C}_6\text{H}_{11} \rightarrow \text{products.}$						
82 ATK/ASC5 ¹⁾	RN	299	(8.55±0.66)(11)			2
¹⁾ CH ₃ ONO/NO/n-Butyl nitrate photolysis. $[CH_3ONO]_0 = (0.9-7.1) \times 10^{14} \text{ molec.cm}^{-3}.$ $[n\text{-Butyl nitrate}] = 2.4 \times 10^{13} \text{ molec.cm}^{-3}.$						
OH + CH₃CH₂CH(CH₃)ONO₂ → products						
Hydroxyl + Nitric acid 1-methylpropyl ester (s-Butyl nitrate)						
82 ATK/ASC5 ¹⁾	RL	299	(9.1±1.3)(-2)			2/2
$k_{ref}: OH + \text{C}_6\text{H}_{11} \rightarrow \text{products.}$						
82 ATK/ASC5 ¹⁾	RN	299	(4.15±0.60)(11)			2
¹⁾ CH ₃ ONO/NO/s-Butyl nitrate photolysis. $[CH_3ONO]_0 = (0.9-7.1) \times 10^{14} \text{ molec.cm}^{-3}.$ $[s\text{-Butyl nitrate}] = 2.4 \times 10^{13} \text{ molec.cm}^{-3}.$						


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH₃CH₂)₂NOH → H₂O + [C₄H₁₀NO]						
Hydroxyl + Ethanamine, N-ethyl-N-hydroxy-						
77 GOR/LII Electron pulse. P(Total) = 760 torr.	EX	308	6.1(13)			2
OH + CH₂=C(CH₃)CH=CH₂ → products						
Hydroxyl + 1,3-Butadiene-, 2-methyl- (Isoprene)						
80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas-chromatography. Same data given on 80 COX. [NO] = NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm.	RN	300	4.46(13)			2
82 ATK/ASC2 ¹⁾ k _{ref} : OH + CH ₃ CH=CH ₂ → products.	RL	299	(3.81±0.17)			2/2
82 ATK/ASC2 ¹⁾ ¹⁾ CH ₃ ONO/NO/Isoprene/Propene photolysis. [CH ₃ ONO] ₀ = (9.5-3.5) × 10 ¹⁴ molec. cm ⁻³ . [Isoprene] = (1.2-2.4) × 10 ¹³ molec. cm ⁻³ . P(Total) = 735 torr.	RN	299	(5.78±0.20)(13)			2
82 KLE/HAR OH generated by flash-photolysis of H ₂ O in Ar. Resonance-fluorescence. P(Total) = 50 torr.	EX	297-424	1.42(13)	0	-409±27	2
OH + CH₃CH₂CH₂CH=CH₂ → H₂O + CH₃CH₂CHCH=CH₂ (a)						
→ CH ₃ CH ₂ CH ₂ CH(OH)CH ₂ (b)						
→ CH ₃ CH ₂ CH ₂ CHCH ₂ OH (c)						
Hydroxyl + 1-Pentene						
82 BIE/HAR ¹⁾ k _a /(k _a + k _b + k _c).	RL	298	(1.3±0.5)(-1)			2/2
82 BIE/HAR ¹⁾ k _a /(k _a + k _b + k _c). P(Total) ~ 2 torr. (Ar)	EX	298	(1.75±0.24)(13)			2
82 BIE/HAR ¹⁾ k _a /(k _a + k _b + k _c). P(Total) = 50 torr. (Ar)	EX	298	(1.73±0.08)(13)			2
¹⁾ Discharge-flow. OH generated by reacting H with NO ₂ . [OH] ₀ = (0.2-2.0) × 10 ¹² molec. cm ⁻³ .						
71 MOR/NIK2 k _{overall} . k _{ref} : CH ₃ CH=CH ₂ + OH → products.	RL	300	2.5			2/2
76 WU/JAP k _{overall} . Pyrex Reactor. P = 760 torr. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.	RL	303	5.6(-1)			2/2
79 NIP/PAR k _{overall} . Flash-photolysis. Resonance-fluorescence.	EX	297	(2.39±0.23)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, . B-B(ref)	k, A k err. units factor
OH + CH₃CH₂CH=CHCH₃ → products						
Hydroxyl + 2-Pentene (Unspecified form)						
71 MOR/NIK2	RL	300	5.3			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
OH + cis-CH₃CH₂CH=CHCH₃ → products						
Hydroxyl + 2-Pentene, (Z)-						
76 WU/JAP	RL	303	1.2			2/2
Cylindrical Pyrex Reactor. P = 760 torr.						
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.						
OH + CH₃CH₂C(CH₃)=CH₂ → products						
Hydroxyl + 1-Butene, 2-methyl-						
71 MOR/NIK2	RL	300	5.3			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
76 WU/JAP	RL	303	1.1			2/2
Cylindrical Pyrex Reactor. P = 760 torr.						
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.						
OH + (CH₃)₂CHCH=CH₂ → products						
Hydroxyl + 1-Butene, 3-methyl-						
77 ATK/PER3	EX	299-424	3.15(12)	0	-533±151	2
77 ATK/PER3	EX	299	(1.87±0.19)(13)			2
OH + (CH₃)₂C=CHCH₃ → products						
Hydroxyl + 2-Butene, 2-methyl-						
71 MOR/NIK2	RL	300	7.0			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
76 ATK/PER1	EX	297-425	2.217(13)	0	-226±201	2
76 ATK/PER1	EX	298	(4.70±0.48)(13)			2
78 ATK/PIT2	EX	299-441	1.15(13)	0	-450±15 1	2
Flash-photolysis. NO ₂ chemiluminescence.						
78 PIT/ATK	EX	298	(4.70±0.54)(13)			2
Flash-photolysis. Resonance-fluorescence.						
P ~ (15-650) torr.						
82 ATK/ASC2 ¹)	RL	299	(3.43±0.13)			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
82 ATK/ASC2 ¹)	RN	299	(5.20±0.20)(13)			2
¹) CH ₃ ONO/NO/2-Methyl-2-butene/Propane photolysis.						
[2-Methyl-2-butene] = (1.2-2.4) × 10 ¹³ molec.cm ⁻³ .						
[CH ₃ ONO] ₀ = (9.5-3.5) × 10 ¹⁴ molec.cm ⁻³ .						
P(Total) = 735 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH +  → products						
Hydroxyl + Cyclopentane						
82 ATK/ASC2 ¹⁾ k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(7.04±0.07)(-1)			2/2
82 ATK/ASC2 ¹⁾	RN	299	(3.21±0.04)(12)			2
¹⁾ CH ₃ ONO/NO/Cyclohexane/Cyclopentane photolysis. [Cyclopentane] = (1.2-2.4) × 10 ¹³ molec. cm ⁻³ . [CH ₃ ONO] ₀ = (9.5-3.5) × 10 ¹⁴ molec. cm ⁻³ . P(Total) = 735 torr.						
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ → H ₂ O + CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ (a) → H ₂ O + CH ₃ CH ₂ CH ₂ CHCH ₃ (b) → H ₂ O + CH ₃ CH ₂ CHCH ₂ CH ₃ (c)						
Hydroxyl + Pentane						
78 DAR/ATK k _a . Irradiation technique. Computed from an empirical formula.	CO	300	2.35(11)			2
79 BAL/WAL1 k _a /k _{ref} . A and B recalculated from a given empirical formula. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	1.28	0	-1070	2/2
78 DAR/ATK k _b . Irradiation technique. Computed from an empirical formula.	CO	300	1.40(12)			2
79 BAL/WAL1 k _b /k _{ref} . A and B recalculated from a given empirical formula. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	6.92(-1)	0	-1820	2/2
78 DAR/ATK k _c . Irradiation technique. Computed from an empirical formula.	CO	300	6.99(11)			2
79 BAL/WAL1 k _c /k _{ref} . A and B recalculated from a given empirical formula. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	753-773	3.46(-1)	0	-1820	2/2
76 WU/JAP k _a + k _b + k _c . Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	1.2(-1)			2/2
78 DAR/ATK k _a + k _b + k _c . Irradiation technique.	EX	300	(2.25±0.08)(12)			2
80 COX/DER1	RN	300	3.01(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$k_a + k_b + k_c$. HONO photosensitized oxidation in synthetic air. $[\text{NO}] = [\text{NO}_2] = (0.3-3.0)$ ppm. $[\text{HONO}] = (3-20)$ ppm. Same data given in 80 COX.						
82 ATK/ASC3 ¹⁾	RL	299	$(4.53 \pm 0.07)(-1)$			2/2
$(k_a + k_b + k_c)/k_{\text{ref}}$. k_{ref} : $\text{OH} + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{products}$.						
82 ATK/ASC3 ¹⁾	RN	299	$(2.49 \pm 0.05)(12)$			2
$k_a + k_b + k_c$. ¹⁾ Photolysis of $\text{CH}_3\text{ONO}/\text{NO}/\text{Pentane}$ mixtures. $[\text{CH}_3\text{ONO}]_0 = (2.1-4.0) \times 10^{14}$ molec. cm^{-3} . $[\text{Pentane}] = (1.2-2.4) \times 10^{13}$ molec. cm^{-3} . $P(\text{Total}) = 735$ torr.						
$\text{OH} + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \rightarrow \text{H}_2\text{O} + \text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{H}_2\text{O} + (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2$ (b) $\rightarrow \text{H}_2\text{O} + (\text{CH}_3)_2\text{CHCHCH}_3$ (c) $\rightarrow \text{H}_2\text{O} + (\text{CH}_3)_2\text{CCH}_2\text{CH}_3$ (d)						
Hydroxyl + Butane, 2-methyl- (Isopentane)						
78 DAR/ATK ¹⁾	CO	300	2.35(11)			2
k_a .						
78 DAR/ATK ¹⁾	CO	300	1.17(11)			2
k_b .						
78 DAR/ATK ¹⁾	CO	300	6.99(11)			2
k_c .						
78 DAR/ATK ¹⁾	CO	300	1.26(12)			2
k_d .						
¹⁾ Irradiation. k computed from an empirical formula.						
79 BAL/WAL1 ²⁾	RL	753-773	1.28	0	-1070	2/2
k_a/k_{ref} .						
79 BAL/WAL1 ²⁾	RL	753-773	6.42(-1)	0	-1070	2/2
k_b/k_{ref} .						
79 BAL/WAL1 ²⁾	RL	753-773	3.46(-1)	0	-1820	2/2
k_c/k_{ref} .						
79 BAL/WAL1 ²⁾	RL	753-773	2.73(-1)	0	-2060	2/2
k_d/k_{ref} .						
²⁾ A and B recalculated from a empirical formula.						
k_{ref} : $\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$.						
76 LLO/DAR2	RL	305	1.10			2/2
$(k_a + k_b + k_c + k_d)/k_{\text{ref}}$.						
k_{ref} : $\text{OH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}$.						
76 LLO/DAR2	RN	305	$(2.0 \pm 0.4)(12)$			2
$k_a + k_b + k_c + k_d$.						




4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
78 DAR/ATK $k_a + k_b + k_c + k_d$. Irradiation technique.	EX	300	(2.28±0.04)(12)			2
80 COX/DER1 $k_a + k_b + k_c + k_d$. HONO photosensitized oxidation in synthetic air. [NO] = [NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm. Same data given in 80 COX.	RN	300	2.11(12)			2
OH + (CH₃)₄C → H₂O + (CH₃)₃CCH₂						
Hydroxyl + Propane, 2,2-dimethyl- (Neopentane)						
71 BAK/BAL ¹⁾	RL	753	(1.60±0.16)(1)			2/2
76 BAK/BAL ¹⁾	RL	753	(1.0±0.1)(1)			2/2
¹⁾ k_{ref} : OH + H ₂ → H ₂ O + H.						
76 BAK/BAL	ES	753	(3.9±0.4)(12)			2
78 DAR/ATK ¹⁾	EX	300	(6.3±1.0)(11)			2
78 DAR/ATK ¹⁾	CO	300	4.70(11)			2
Calculation using an empirical formula.						
¹⁾ Irradiation technique.						
79 BAL/WAL1	RL	753-773	2.57	0	-1070	2/2
A and B recalculated from a empirical formula.						
k_{ref} : OH + H ₂ → H ₂ O + H.						
80 PAR/NIP	EX	297	(5.48±0.59)(11)			2
Flash-photolysis. Resonance-absorption.						
82 ATK/ASC2 ¹⁾	RL	299	(1.35±0.07)(-1)			2/2
k_{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.						
82 ATK/ASC2 ¹⁾	RN	299	(4.64±0.30)(11)			2
¹⁾ CH ₃ ONO/NO/Neopentane photolysis.						
[Neopentane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ .						
[CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ .						
P(Total) = 735 torr.						
OH + CH₃CH₂CH₂CH₂CHO → H₂O + CH₃CH₂CH₂CH₂CO (a)						
→ H ₂ O + CH ₃ CH ₂ CH ₂ CHCHO (b)						
→ H ₂ O + CH ₃ CH ₂ CHCH ₂ CHO (c)						
→ H ₂ O + CH ₃ CHCH ₂ CH ₂ CHO (d)						
→ H ₂ O + CH ₂ CH ₂ CH ₂ CH ₂ CHO (e)						
Hydroxyl + Pentanal						
81 AUD/BAU ¹⁾	RL	298	(8.8±1.1)(-1)			2/2
(k _a + k _b + k _c + k _d + k _e)/k _{ref} .						
k_{ref} : OH + CH ₃ CHO → products.						
81 AUD/BAU ¹⁾	RN	298	(8.3±1.0)(12)			2
$k_a + k_b + k_c + k_d + k_e$.						
¹⁾ Linear, boric-acid-coated flow tube. Channel						
(a) is predominant. P(Total) = 299 torr.						



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 KER/SHE ²⁾ (k _a + k _b + k _c + k _d + k _e)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(3.24±0.49)			2/2
81 KER/SHE ²⁾ k _a + k _b + k _c + k _d + k _e . ²⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(1.57±0.24)(13)			2
OH + (CH ₃) ₂ CHCH ₂ CHO → H ₂ O + (CH ₃) ₂ CHCH ₂ CO (a) → H ₂ O + (CH ₃) ₂ CHCHO (b) → H ₂ O + (CH ₃) ₂ CCH ₂ CHO (c) → H ₂ O + CH ₂ CH(CH ₃)CH ₂ CHO (d)						
Hydroxyl + Butanal, 3-methyl-						
81 AUD/BAU ¹⁾ (k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₃ CHO → products.	RL	298	(1.18±0.13)			2/2
81 AUD/BAU ¹⁾ k _a + k _b + k _c + k _d . ¹⁾ Boric-acid-coated flow tube. Channel (a) is predominant. P(Total) = 299 torr.	RN	298	(1.11±0.12)(13)			2
81 KER/SHE ²⁾ (k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(3.39±0.10)			2/2
81 KER/SHE ²⁾ k _a + k _b + k _c + k _d . ²⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(1.63±0.06)(13)			2
OH + (CH ₃) ₃ CCHO → H ₂ O + (CH ₃) ₃ CCO (a) → H ₂ O + CH ₂ C(CH ₃) ₂ CHO (b)						
Hydroxyl + Propanal, 2,2-dimethyl-						
81 AUD/BAU ¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : OH + CH ₃ CHO → products.	RL	298	(5.4±0.6)(-1)			2/2
81 AUD/BAU ¹⁾ k _a + k _b . ¹⁾ Boric-acid-coated flow tube. Channel (a) is predominant. P(Total) = 299 torr.	RN	298	(5.1±0.5)(12)			2
81 KER/SHE ²⁾ (k _a + k _b)/k _{ref} . k _{ref} : OH + CH ₂ =CH ₂ → products.	RL	298	(2.63±0.73)			2/2
81 KER/SHE ²⁾ k _a + k _b . ²⁾ HONO/Synthetic air/Ethene/aldehyde photolysis.	RN	298	(1.26±0.36)(13)			2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₃C(O)CH₂CH₂CH₃ → products						
Hydroxyl + 2-Pentanone						
82 ATK/ASC4 ¹⁾	RL	299	(6.26±0.18)(-1)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC4 ¹⁾	RN	299	(2.85±0.08)(12)			2
¹⁾ CH ₃ ONO/NO/2-Pentanone photolysis. [2-Pentanone] = (1.2-2.4) × 10 ¹⁴ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-4.0) × 10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + (CH₃CH₂)₂CO → products						
Hydroxyl + 3-Pentanone						
82 ATK/ASC4 ¹⁾	RL	299	(2.45±0.44)(-1)			2/2
k _{ref} : OH +  → products.						
82 ATK/ASC4 ¹⁾	RN	299	(1.11±0.20)(12)			2
¹⁾ CH ₃ ONO/NO/2-Pentanone photolysis. [3-Pentanone] = (1.2-2.4) × 10 ¹⁴ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-4.0) × 10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + CH₃C(O)OCH₂CH₂CH₃ → products						
Hydroxyl + Acetic acid propyl ester (n-Propyl nitrate)						
77 WIN/LLO	RL	305	8.5(-2)			2/2
k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
77 WIN/LLO	RN	305	(2.6±0.5)(12)			2
OH + CH₃CH₂C(O)OCH₂CH₃ → products						
Hydroxyl + Propanoic acid ethyl ester						
78 CAM/PAR	EX	292	(1.06±0.15)(12)			2
Reaction of ester vapor with OH in Pyrex vessel with vacuum system. OH generated by the reaction of a H ₂ O ₂ /NO ₂ /CO mixture. P(Total) = 100 torr.						
OH + CH₃CH₂CH₂CH(CH₃)ONO₂ → products						
Hydroxyl + 2-Pentanol nitrate						
82 ATK/ASC5 ¹⁾	RL	299	(2.47±0.16)(-1)			2/2
k _{ref} : OH +  → products.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC5 ¹⁾ 1) CH ₃ ONO/NO/2-Pentanol nitrate photolysis. [CH ₃ ONO] ₀ = (0.9-7.1) × 10 ¹⁴ molec. cm ⁻³ . [Alkyl nitrate] = 2.4 × 10 ¹³ molec. cm ⁻³ .	RN	299	(1.13 ± 0.07)(12)			2
OH + (CH ₃ CH ₂) ₂ CHONO ₂ → products Hydroxyl + 3-Pentanol nitrate						
82 ATK/ASC5 ¹⁾ k _{ref} : OH +  → products.	RL	299	(1.49 ± 0.26)(-1)			2/2
82 ATK/ASC5 ¹⁾ 1) CH ₃ ONO/NO/3-Pentanol nitrate photolysis. [CH ₃ ONO] ₀ = (0.9-7.1) × 10 ¹⁴ molec. cm ⁻³ . [Alkyl nitrate] = 2.4 × 10 ¹³ molec. cm ⁻³ .	RN	299	(6.81 ± 1.20)(11)			2
OH +  → products Hydroxyl + Cyclohexene						
76 DAR/WIN k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	1.53			2/2
76 DAR/WIN	RN	305	(4.7 ± 0.9)(13)			2
76 WU/JAP Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	1.2			2/2
80 COX/DER1 HONO photosensitized oxidation in synthetic air. Gas-chromatography. Same data given in 80 COX. [NO] = NO ₂ = (0.3-3.0) ppm. [HONO] = (3-20) ppm.	RN	298	3.73(13)			2
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH=CH ₂ → products Hydroxyl + 1-Hexene						
76 WU/JAP Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	6.0(-1)			2/2
OH + (CH ₃) ₃ CCH=CH ₂ → products Hydroxyl + 1-Butene, 3,3-dimethyl-						
76 WU/JAP Cylindrical Pyrex Reactor. k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	5.2(-1)			2/2



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH₃)₂C=C(CH₃)₂ → products						
Hydroxyl + 2-Butene, 2,3-dimethyl-						
71 MOR/NIK2	RL	300	9.0			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
77 DAV ¹)	EX	298	(3.42±0.07)(13)			2
78 RAV/WAG ¹)	EX	298	(3.43±0.08)(13)			2
¹) M = He. Flash-photolysis.						
Resonance-fluorescence. P(He) = 20 torr.						
82 ATK/ASC2 ²)	RL	299	(4.28±0.21)			2/2
k _{ref} : OH + CH ₃ CH=CH ₂ → products.						
82 ATK/ASC2 ²)	RN	299	(6.50±0.36)(13)			2
²) CH ₃ ONO/NO/2,3-Dimethyl-2-butene/Propene photolysis.						
[(CH ₃) ₂ C=C(CH ₃) ₂] = (1.2-2.4) × 10 ¹³ molec.cm ⁻³ .						
[CH ₃ ONO] ₀ = (9.5-3.5) × 10 ¹⁴ molec.cm ⁻³ .						
P(Total) = 735 torr.						
OH +  → products						
Hydroxyl + Cyclohexane						
74 GOR/VOL	RL	298	4.48(1)			2/2
74 GOR/VOL	RN	298	(4.04±0.90)(12)			2
76 WU/JAP	RL	303	1.2(-1)			2/2
Cylindrical Pyrex Reactor.						
k _{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products.						
P = 760 torr.						
82 ATK/ASC2 ¹)	RL	299	(1.32±0.04)			2/2
k _{ref} : OH + CH ₃ (CH ₂)CH ₃ → products.						
82 ATK/ASC2 ¹)	RN	299	(4.53±0.16)			2
¹) CH ₃ ONO/NO/Cyclohexane/Hexane photolysis.						
[Cyclohexane] = (1.2-2.4) × 10 ¹³ molec.cm ⁻³ .						
[CH ₃ ONO] ₀ = (9.5-3.5) × 10 ¹⁴ molec.cm ⁻³ .						
P(Total) = 735 torr.						
OH + CH₃(CH₂)₄CH₃ → H₂O + CH₃(CH₂)₄CH₂ (a)						
→ H₂O + CH₃(CH₂)₃CHCH₃ (b)						
→ H₂O + CH₃(CH₂)₂CH(CH₂)₂CH₃ (c)						
Hydroxyl + Hexane						
76 LLO/DAR2	RL	305	2.09			2/2
(k _a + k _b + k _c)/k _{ref} .						
k _{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.						
76 CAM/MCL ¹)	EX	292	(3.3±0.2)(12)			2
76 LLO/DAR2 ¹)	RN	305	(3.8±0.8)(12)			2



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 WU/JAP ¹⁾ Cylindrical Pyrex Reactor. k_{ref} : OH + cis-CH ₃ CH=CHCH ₃ → products. P = 760 torr.	RL	303	1.1(-1)			2/2
82 ATK/ASC2 ¹⁾ CH ₃ ONO/NO/Hexane photolysis. [CH ₃ ONO] ₀ = (9.5-3.5) × 10 ¹⁴ molec. cm ⁻³ . [Hexane] = (1.2-2.4) × 10 ¹³ molec. cm ⁻³ . P(Total) = 735 torr.	EX	299	(3.43 ± 0.05)(12)			2
¹⁾ $k_a + k_b + k_c$.						
OH + (CH ₃) ₂ CHCH ₂ CH ₂ CH ₃ → H ₂ O + (CH ₃) ₂ CHCH ₂ CH ₂ CH ₂ (a)						
→ H ₂ O + (CH ₃) ₂ CHCH ₂ CH ₂ CH ₃ (b)						
→ H ₂ O + (CH ₃) ₂ CHCHCH ₂ CH ₃ (c)						
→ H ₂ O + (CH ₃) ₂ CCH ₂ CH ₂ CH ₃ (d)						
→ H ₂ O + CH ₂ CH(CH ₃)CH ₂ CH ₂ CH ₃ (e)						
Hydroxyl + Pentane, 2-methyl-						
76 LLO/DAR2 ($k_a + k_b + k_c + k_d + k_e$)/ k_{ref} . k_{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	305	1.77			2/2
76 LLO/DAR2 ¹⁾	RN	305	(3.2 ± 0.6)(12)			2
80 COX/DER1 ¹⁾ HONO photosensitized oxidation in synthetic air. Gas-chromatography. [NO] = NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm. Same data given in 80 COX.	RN	298	3.01(12)			2
¹⁾ $k_a + k_b + k_c + k_d + k_e$.						
OH + CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₃						
→ H ₂ O + CH ₃ CH ₂ CH(CH ₃)CH ₂ CH ₂ (a)						
→ H ₂ O + CH ₃ CH ₂ CH(CH ₃)CHCH ₃ (b)						
→ H ₂ O + CH ₃ CH ₂ C(CH ₃)CH ₂ CH ₃ (c)						
→ H ₂ O + CH ₃ CH ₂ CH(CH ₂)CH ₂ CH ₃ (d)						
→ H ₂ O + CH ₃ CHCH(CH ₃)CH ₂ CH ₃ (e)						
→ H ₂ O + CH ₂ CH ₂ CH(CH ₃)CH ₂ CH ₃ (f)						
Hydroxyl + Pentane, 3-methyl-						
76 LLO/DAR2 ($k_a + k_b + k_c + k_d + k_e + k_f$)/ k_{ref} . k_{ref} : OH + CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	305	2.40			2/2
76 LLO/DAR2 $k_a + k_b + k_c + k_d + k_e + k_f$.	RN	305	(4.3 ± 0.9)(12)			2




4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH ₃) ₂ CHCH(CH ₃) ₂ → H ₂ O + CH ₂ CH(CH ₃)CH(CH ₃) ₂ (a) → H ₂ O + (CH ₃) ₂ CCH(CH ₃) ₂ (b)						
Hydroxyl + Butane, 2,3-dimethyl-						
78 DAR/ATK ¹) k _a . Computed from an empirical formula.	CO	300	4.70(11)			2
78 DAR/ATK ¹) k _b . Computed from an empirical formula.	CO	300	2.53(12)			2
¹) Irradiation technique.						
76 DAR/WIN (k _a + k _b)/k _{ref} . k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	1.0(-1)			2/2
76 DAR/WIN k _a + k _b .	RN	305	(3.1±0.6)(12)			2
78 DAR/ATK k _a + k _b . Irradiation technique.	EX	300	(3.42±0.17)(12)			2
80 COX/DER1 k _a + k _b . HONO photosensitized oxidation in synthetic air. [NO] = [NO ₂] = (0.3-3.0) ppm. [HONO] = (3-20) ppm. Same data given in 80 COX.	RN	298	2.29(12)			2
82 ATK/ASC2 ²) (k _a + k _b)/k _{ref} . k _{ref} : OH +  → products.	RL	299	(8.27±0.04)(-1)			2/2
82 ATK/ASC2 ²) k _a + k _b .	RN	299	(3.77±0.04)(12)			2
²) CH ₃ ONO/NO/2,3-Dimethylbutane/Cyclohexane photolysis. [CH ₃ ONO] ₀ = (9.5-3.5)×10 ¹⁴ molec.cm ⁻³ . [2,3-Dimethylbutane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + CH ₃ C(O)CH ₂ CH ₂ CH ₂ CH ₃ → products						
Hydroxyl + 2-Hexanone						
82 ATK/ASC4 ¹) k _{ref} : OH +  → products.	RL	299	(1.21±0.08)			2/2
82 ATK/ASC4 ¹) ¹) CH ₃ ONO/NO/2-Hexanone photolysis. [2-Hexanone] = (1.2-2.4)×10 ¹⁴ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(5.52±0.37)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₃CH₂C(O)CH₂CH₂CH₃ → products						
Hydroxyl + 3-Hexanone						
82 ATK/ASC4 ¹⁾	RL	299	(9.19±0.38)(-1)			2/2
k_{ref} : OH +  → products.						
82 ATK/ASC4 ¹⁾	RN	299	(4.19±0.17)(12)			2
¹⁾ CH ₃ ONO/NO/3-Hexanone photolysis. torr. [3-Hexanone] = (1.3-2.4)×10 ¹⁴ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + CH₃C(O)CH₂CH(CH₃)₂ → products						
Hydroxyl + 2-Pentanone, 4-methyl-						
76 WIN/LLO	RL	305	3.0(-1)			2/2
k_{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 WIN/LLO	RN	305	(9.0±3.0)(12)			2
80 COX/DER1	RN	300	7.47(12)			2
HONO photosensitized oxidation in synthetic air. Gas-chromatography. [NO] = NO ₂ = (0.3-3.0) ppm. [HONO] = (3-20) ppm. Same data given on 80 COX.						
81 COX/PAT	EX	296	(7.83±0.18)(12)			2
HONO/N ₂ /O ₂ /4-Methyl-2-pentanone photolysis. P = 760 torr.						
82 ATK/ASC4 ¹⁾	RL	299	(1.91±0.09)			2/2
k_{ref} : OH +  → products.						
82 ATK/ASC4 ¹⁾	RN	299	(8.73±0.42)(12)			2
¹⁾ CH ₃ ONO/NO/4-Methyl-2-Pentanone photolysis. [CH ₃ ONO] ₀ = (0.9-4.0)×10 ¹⁴ molec.cm ⁻³ . [4-Methyl-2-Pentanone] = (1.3-2.4)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + CH₃C(O)OCH(CH₃)CH₂CH₃ → products						
Hydroxyl + Acetic acid 1-methylpropyl ester (s-Butyl acetate)						
77 WIN/LLO	RL	305	1.1(-1)			2/2
k_{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
77 WIN/LLO	RN	305	(3.4±0.7)(12)			2




4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH₃CH₂CH₂OCH₂CH₂CH₃ → products						
Hydroxyl + Propane, 1,1'-oxybis- (di-n-Propyl ether)						
76 LLO/DAR1	RL	305	3.4(-1)			2/2
k_{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 LLO/DAR1	RN	305	(1.04±0.21)(13)			2
OH + CH₃CH₂CH₂CH₂CH(CH₃)ONO₂ → products						
Hydroxyl + 2-Hexanol nitrate						
82 ATK/ASC5 ¹⁾	RL	299	(4.22±0.20)(-1)			2/2
k_{ref} : OH +  → products.						
82 ATK/ASC5 ¹⁾	RN	299	(1.92±0.09)(12)			2
¹⁾ CH ₃ ONO/NO/2-Hexanol nitrate photolysis. [Alkyl nitrate] = 2.4x10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-7.1)x10 ¹⁴ molec.cm ⁻³ .						
OH + CH₃CH₂CH₂CH(CH₂CH₃)ONO₂ → products						
Hydroxyl + 3-Hexanol nitrate						
82 ATK/ASC5 ¹⁾	RL	299	(3.59±0.28)(-1)			2/2
k_{ref} : OH +  → products.						
82 ATK/ASC5 ¹⁾	RN	299	(1.64±0.13)(12)			2
¹⁾ CH ₃ ONO/NO/3-Hexanol nitrate photolysis. [Alkyl nitrate] = 2.4x10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-7.1)x10 ¹⁴ molec.cm ⁻³ .						
OH +  → products						
Hydroxyl + Cyclohexene, 1-methyl-						
76 DAR/WIN	RL	305	1.91			2/2
k_{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 DAR/WIN	RN	305	(5.8±1.2)(13)			2
OH + CH₃CH₂CH₂CH₂CH₂CH=CH₂ → products						
Hydroxyl + 1-Heptene						
76 DAR/WIN	RL	305	7.3(-1)			2/2
k_{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.						
76 DAR/WIN	RN	305	(2.2±0.5)(13)			2


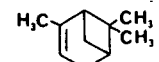
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + CH ₃ (CH ₂) ₅ CH ₃ → H ₂ O + CH ₃ (CH ₂) ₅ CH ₂ (a)						
→ H ₂ O + CH ₃ (CH ₂) ₄ CHCH ₃ (b)						
→ H ₂ O + CH ₃ (CH ₂) ₃ CHCH ₂ CH ₃ (c)						
→ H ₂ O + CH ₃ (CH ₂) ₂ CH(CH ₂) ₂ CH ₃ (d)						
Hydroxyl + Heptane						
82 ATK/ASC3 ¹⁾ (k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(1.28±0.02)			2/2
82 ATK/ASC3 ¹⁾ k _a + k _b + k _c + k _d .	RN	299	(4.40±0.10)(12)			2
¹⁾ CH ₃ ONO/NO/Heptane photolysis. [Heptane] = (1.2-2.4)×10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (2.1-4.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + (CH ₃) ₃ CCH(CH ₃) ₂ → H ₂ O + CH ₂ C(CH ₃) ₂ CH(CH ₃) ₂ (a)						
→ H ₂ O + (CH ₃) ₃ CCH(CH ₃)CH ₂ (b)						
→ H ₂ O + (CH ₃) ₃ CC(CH ₃) ₂ (c)						
Hydroxyl + Butane, 2,2,3-trimethyl-						
81 BAL/WAL2 (k _a + k _b)/k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio. Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ , in aged boric-acid-coated reaction vessels. P(2,2,3-Trimethylbutane) = 5 torr. P(Total) = 500 torr.	RL	753	6.7			2/2
76 DAR/WIN (k _a + k _b + k _c)/k _{ref} . k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	7.4(-2)			2/2
76 DAR/WIN k _a + k _b + k _c .	RN	305	(2.3±0.5)(12)			2
81 BAL/WAL2 ¹⁾ (k _a + k _b + k _c)/k _{ref} . Optimization. k _{ref} : OH + H ₂ → H ₂ O + H.	RL	300-500	(1.22±0.15)(1)	0	0	2/2
81 BAL/WAL2 ¹⁾ k _a + k _b + k _c .	SE	300-500	(5.92±0.50)(12)	0	217±42	2
81 BAL/WAL2 ¹⁾ k _c /k _{ref} . k _{ref} : OH + H ₂ → H ₂ O + H. Estimated ratio.	RL	753	5.5			2/2
81 BAL/WAL2 ¹⁾ k _c .	ES	300-1500	1.70(12)	0	-115±96	2 1.23
¹⁾ Oxidation of 2,2,3-Trimethylbutane in H ₂ O ₂ mixtures, in aged boric-acid-coated reaction vessels. Gas-chromatography. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.						

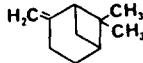
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH + (CH ₃) ₂ CHC(O)CH(CH ₃) ₂ → products Hydroxyl + 3-Pentanone, 2,4-dimethyl- 82 ATK/ASC4 ¹)	RL	299	(7.17±0.54)(-1)			2/2
k _{ref} : OH +  → products. 82 ATK/ASC4 ¹)	RN	299	(3.27±0.24)(12)			2
¹) CH ₃ ONO/NO/2,4-Dimethyl-3-Pentanone photolysis. [2,4-Dimethyl-3-Pentanone] = (1.3-2.4) × 10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr. [CH ₃ ONO] ₀ = (0.9-4.0) × 10 ¹⁴ molec.cm ⁻³ .						
OH + CH ₃ CH ₂ CH ₂ CH ₂ CH(CH ₂ CH ₃)ONO ₂ → products Hydroxyl + 3-Heptanol nitrate 82 ATK/ASC5 ¹)	RL	299	(4.91±0.57)(-1)			2/2
k _{ref} : OH +  → products. 82 ATK/ASC5 ¹)	RN	299	(2.24±0.26)(12)			2
¹) CH ₃ ONO/NO/3-Heptanol nitrate photolysis. [Alkyl nitrate] = 2.4 × 10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-7.1) × 10 ¹⁴ molec.cm ⁻³ .						
OH + CH ₃ (CH ₂) ₆ CH ₃ → H ₂ O + CH ₃ (CH ₂) ₆ CH ₂ (a) → H ₂ O + CH ₃ (CH ₂) ₅ CHCH ₃ (b) → H ₂ O + CH ₃ (CH ₂) ₄ CHCH ₂ CH ₃ (c) → H ₂ O + CH ₃ (CH ₂) ₃ CH(CH ₂) ₂ CH ₃ (d)						
Hydroxyl + Octane 82 ATK/ASC3 ¹)	RL	299	(1.58±0.02)			2/2
(k _a + k _b + k _c + k _d)/k _{ref} . k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products. 82 ATK/ASC3 ¹)	RN	299	(5.43±0.11)(12)			2
k _a + k _b + k _c + k _d . ¹) CH ₃ ONO/NO/Octane photolysis. [Octane] = (1.2-2.4) × 10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (2.1-4.0) × 10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.						
OH + CH ₃ (CH ₂) ₄ CH(CH ₂ CH ₃)ONO ₂ → products Hydroxyl + 3-Octanol nitrate 82 ATK/ASC5 ¹)	RL	299	(5.16±1.05)(-1)			2/2
k _{ref} : OH +  → products.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ATK/ASC5 ¹⁾ ¹⁾ CH ₃ ONO/NO/3-Octanol nitrate photolysis. [Alkyl nitrate] = 2.4x10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (0.9-7.1)x10 ¹⁴ molec.cm ⁻³ .	RN	299	(2.35±0.48)(12)			2
OH + CH ₃ (CH ₂) ₇ CH ₃ → H ₂ O + CH ₃ (CH ₂) ₇ CH ₂ (a) → H ₂ O + CH ₃ (CH ₂) ₆ CHCH ₃ (b) → H ₂ O + CH ₃ (CH ₂) ₅ CHCH ₂ CH ₃ (c) → H ₂ O + CH ₃ (CH ₂) ₄ CH(CH ₂) ₂ CH ₃ (d) → H ₂ O + CH ₃ (CH ₂) ₃ CH(CH ₂) ₃ CH ₃ (e)						
Hydroxyl + Nonane						
82 ATK/ASC3 ¹⁾ (k _a + k _b + k _c + k _d + k _e)/k _{ref} . k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(1.87±0.05)			2/2
82 ATK/ASC3 ¹⁾ k _a + k _b + k _c + k _d + k _e . ¹⁾ CH ₃ ONO/NO/Nonane photolysis. [Nonane] = (1.2-2.4)x10 ¹³ molec.cm ⁻³ . [CH ₃ ONO] ₀ = (2.1-4.0)x10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr.	RN	299	(6.44±0.24)(12)			2
OH + (CH ₃) ₂ CHCH ₂ COCH ₂ (CH ₃) ₂ → products						
Hydroxyl + 4-Heptanone, 2,6-dimethyl-						
76 WIN/LLO k _{ref} : OH + (CH ₃) ₂ C=CH ₂ → products.	RL	305	5.0(-1)			2/2
76 WIN/LLO	RN	305	(1.5±0.5)(13)			2
82 ATK/ASC4 ¹⁾ k _{ref} : OH +  → products.	RL	299	(3.66±0.19)			2/2
82 ATK/ASC4 ¹⁾ ¹⁾ CH ₃ ONO/NO/2,6-Dimethyl-4-Heptanone photolysis. [2,6-Dimethyl-4-Hexanone] = (1.3-2.4)x10 ¹⁴ molec.cm ⁻³ . P(Total) = 735 torr. [CH ₃ ONO] ₀ = (0.9-4.0)x10 ¹⁴ molec.cm ⁻³ .	RN	299	(1.67±0.09)(12)			2
OH +  → products						
Hydroxyl + Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl- (α-Pinene)						
82 KLE/HAR OH generated by H ₂ O flash-photolysis. Resonance-fluorescence. P(Total) = 50 torr. (Ar)	EX	297-424	8.25(12)	0	-446±75	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
OH +  → products						
Hydroxyl + Bicyclo[3.1.1]heptane, 6,6-dimethyl- 2-methylene- (β -Pinene)						
82 KLE/HAR OH generated by the H ₂ O flash-photolysis. Resonance-fluorescence. P(Total) = 50 torr. (Ar)	EX	297-424	1.42(13)	0	-358±58	2
OH + CH ₃ (CH ₂) ₈ CH ₃ → H ₂ O + CH ₃ (CH ₂) ₈ CH ₂ (a) → H ₂ O + CH ₃ (CH ₂) ₇ CHCH ₃ (b) → H ₂ O + CH ₃ (CH ₂) ₆ CHCH ₂ CH ₃ (c) → H ₂ O + CH ₃ (CH ₂) ₅ CH(CH ₂) ₂ CH ₃ (d) → H ₂ O + CH ₃ (CH ₂) ₄ CH(CH ₂) ₃ CH ₃ (e)						
Hydroxyl + Decane						
82 ATK/ASC3 ¹⁾ (k _a + k _b + k _c + k _d + k _e)/k _{ref} . k _{ref} : OH + CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	299	(2.00±0.09)			2/2
82 ATK/ASC3 ¹⁾ k _a + k _b + k _c + k _d + k _e .	RN	299	(6.87±0.36)(12)			2
1) CH ₃ ONO/NO/Decane photolysis. P(Total) = 735 torr. [CH ₃ ONO] ₀ = (2.1-4.0) × 10 ¹⁴ molec.cm ⁻³ . [Decane] = (1.2-2.4) × 10 ¹³ molec.cm ⁻³ .						
HO ₂ + O ₃ → OH + O ₂ + O ₂						
Hydroperoxo + Ozone						
73 AND/KAU2 Upper-limit k.	EX	220-450	≤3.01(9)			2
73 DEM	EX	300	1.81(9)			2
73 SIM/HEI3	RN	225-298	1.98(10)	0	1007	2
74 DEM/TSC	ES	273-342	1.20(11)	0	1560±252	2 2.0
79 SU/CAL1 Cl ₂ /O ₃ /H ₂ photolysis in O ₂ /N ₂ . FTIR-, and IR- Spectroscopy. Upper-limit k. P(Total) = 700 torr.	ES	298	≤(1.33±0.66)(9)			2
80 ZAH/HOW Discharge-flow. Laser magnetic resonance.	EX	245-365	(8.43±2.41)(9)	0	580±100	2
HO ₂ + HO ₂ (+ M) → H ₂ O ₂ + O ₂ (+ M)						
Hydroperoxo						
72 HOC/GHO	EX	298	(5.7±0.5)(12)			2
72 PAU/JOH	EX	295	(2.17±0.30)(12)			2
75 HAM	EX	298	1.90(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 HAM/LII ¹⁾	EX	298	1.51(12)			2	1.20
77 HAM/LII ¹⁾	RL	298	2.83			2/2	
k _{ref} : DO ₂ + DO ₂ → H ₂ O ₂ + O ₂ .							
77 HAM/LII ¹⁾	EX	298	1.51(12)			2	
¹⁾ Electron pulse radiolysis and Kinetic Spectrometry. P(H ₂) = 2 atm. P(O ₂) = 5 torr.							
78 COX ²⁾	EX	273	2.05(12)			2	
78 COX ²⁾	EX	298	(1.39±0.18)(12)			2	
78 COX ²⁾	EX	338	9.03(11)			2	
²⁾ Cl ₂ /H ₂ /NO ₂ photolysis in N ₂ /O ₂ . P = 1 atm.							
79 BUR/CLI	EX	298	≤7.23(11)			2	
Discharge-flow. Upper-limit k.							
79 COX/BUR	EX	273-339	(2.29±0.84)(10)	0	-1250±200	2	
UV-Absorption spectrometry. P = (3-760) torr. k dependent on P(H ₂ O) and increasing with T. Negative values of E _a and pressure effects discussed in terms of a complex forming mechanism.							
79 GRA/WIN	EX	300	2.29(12)			2	2.0
Thermolysis of HO ₂ NO ₂ . P(Total) = 760 torr.							
79 LII/GOR	EX	276-400	(6.87±0.96)(10)	0	-1057±45	2	
Pulse-radiolysis. Kinetic Spectrophotometry.							
79 THR/WIL ³⁾	EX	298	(1.75±0.72)(11)			2	
P(He) = 2 torr.							
79 THR/WIL ³⁾	EX	298	(2.59±1.08)(11)			2	
P(He) = 3 torr.							
79 THR/WIL ³⁾	EX	298	(3.31±0.84)(11)			2	
P(He) = 4 torr.							
79 THR/WIL ³⁾	EX	298	(4.46±1.99)(11)			2	
P(Ar) = 2.2 torr.							
³⁾ Laser magnetic-resonance spectroscopy in a flow-reactor.							
80 HOC/SWO2	EX	296	(4.0±0.7)(12)			2	
H ₂ O flash-photolysis in presence of O ₂ and CO (or He). P = 760 torr.							
80 LII/GOR1 ⁴⁾	ES	290-400	(5.36±0.18)(10)	0	-1057	2	
80 LII/GOR1 ⁴⁾	ES	298	1.87(12)			2	
⁴⁾ Electron pulse-radiolysis. Kinetic spectrophotometry. P(Total) = 1200 torr.							
81 BUR/COX ⁵⁾	EX	308	(1.25±0.12)(12)			2	
P(H ₂ O) = 0							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 BUR/COX ⁵) P(H ₂ O) = 3.0 torr.	EX	308	(1.33±0.12)(12)				2
81 BUR/COX ⁵) P(H ₂ O) = 0	EX	348	(8.07±0.90)(11)				2
81 BUR/COX ⁵) P(H ₂ O) = 10.5 torr.	EX	348	(9.52±0.90)(11)				2
⁵) O ₃ /H ₂ O/O ₂ /N ₂ (or He) photolysis. Molecular Modulation. P(Total) = 760 torr.							
81 LII/SAU Pulse-radiolysis. k estimated in terms of a complex-forming mechanism.	ES	298-373	(5.54±0.12)(10)	0	-1057		2
82 PAT/PIL HO ₂ generated by the CH ₃ OH/O ₂ /Cl ₂ flash-photolysis in N ₂ . P(CH ₃ OH) ~ P(Cl ₂) ~ 1.5 torr. P(Total) = 700 torr. P(O ₂) ~ 5 torr.	EX	298-510	(2.49±0.69)(11)	0	-630±115		2
82 SAN/PET ⁶) HO ₂ generated by the Cl ₂ /CH ₃ OH/O ₂ photolysis.	EX	298	(9.64±1.20)(11)				2
82 SAN/PET ⁶) HO ₂ generated by the Cl ₂ /H ₂ /O ₂ photolysis. P(H ₂) = 130 torr. P(O ₂) = 560 torr.	EX	298	(1.54±0.11)(12)				2
⁶) Flash-photolysis. UV-absorption spectrometry.							
82 SIM/HEI ⁷) Limiting low-pressure k.	EX	296	(8.43±1.20)(11)				2
82 SIM/HEI ⁷) P(N ₂) = 760 torr.	EX	296	(1.51±0.06)(12)				2
⁷) Flash-photolysis. UV-absorption spectrometry. HO ₂ generated by the Cl ₂ /CH ₃ OH/O ₂ photolysis. M = He, or N ₂ . P-dependent from 5 to 770 torr. [HO ₂] = (1.3-3.3) × 10 ¹⁴ molec.cm ⁻³ .							
82 THR/TYN2 Flash-photolysis combined with tunable-diode Laser-spectroscopy. HO ₂ generated the Cl ₂ /CH ₃ OH/O ₂ photolysis. k is P-independent within the given range. [HO ₂] ₀ = (0.58-1.20) × 10 ¹⁵ molec.cm ⁻³ . P(Total) = (7-20) torr.	EX	298-358	1.44(11)	0	-560		2
82 SAN/PET M = He. M-efficiencies relative to He are: 1.0(He), 1.61(Ar), 1.67(O ₂), 1.33(N ₂), 2.75(SF ₆). Flash-photolysis. UV-Absorption-spectroscopy. HO ₂ generated by photolysing Cl ₂ /CH ₃ OH/O ₂ . Limiting low-pressure k's within the (100-700) torr. range.	EX	298	8.34(15)				3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
DO₂ + DO₂ → D₂O₂ + O₂							
Hydroperoxo-d₂							
77 HAM/LII	EX	298	5.32(11)			2	1.20
77 HAM/LII	EX	298	5.32(12)			2	
Electro-n pulse radiolysis. Kinetic spectrophotometry. P(H ₂) = 2 atm. P(O ₂) = 5 torr.							
82 SAN/PET	EX	298	(4.22±0.24)(11)			2	
HO ₂ generated by the Cl ₂ /D ₂ /O ₂ flash-photolysis. UV-absorption spectrometry. P = 700 torr.							
HO₂ + SO₂ (+ M) → OH + SO₃ (+ M) (a)							
→ HO₂SO₂ (+ M) (b)							
Hydroperoxo + Sulfur dioxide							
73 PAY/STI ¹⁾	RN	300	(5.24±0.18)(8)			2	
79 BUR/CLI ¹⁾	EX	298	≤1.20(7)			2	
Discharge-flow. Upper-limit k.							
79 GRA/WIN ¹⁾	EX	300	≤6.02(5)			2	
HO ₂ NO ₂ thermolysis. Upper-limit k. P(Total) = 760 torr.							
¹⁾ k _a .							
79 BUR/CLI	EX	298	≤1.45(14)			3	
k _b . M = He. Discharge-flow. Upper-limit k.							
HO₂ + NO (+ M) → O₂ + HNO (+ M) (a)							
→ OH + NO₂ (+ M) (b)							
→ HONO₂ (+ M) (c)							
Hydroperoxo + Nitrogen oxide (NO)							
79 HOW ¹⁾	EX	271	<1.81(10)			2	
79 HOW ¹⁾	EX	303	<6.02(9)			2	
¹⁾ k _a . Upper-limit k's. Discharge-flow. Laser-Magnetic Resonance.							
74 SIM/HEI2	RL	298	(7.0±1.0)			2/2	
k _b /k _{ref} . k _{ref} : HO ₂ + NO ₂ → HONO + O ₂							
73 PAY/STI ²⁾	ES	300	1.8(11)			2	3.0
73 SIM/HEI1 ²⁾	ES	298	>9.03(10)			2	
Lower-limit k.							
74 HAC/HOY2 ²⁾	EX	298-669	(2.0±1.0)(13)	0	1430	2	
75 COX ²⁾	ES	300	(7.23±1.81)(11)			2	
75 COX/DER1 ²⁾	ES	296	(7.23±1.81)(11)			2	
75 GLA/TRO ²⁾	ES	1350-1700	(4.5±1.0)(12)			2	
75 HAC/HOY ²⁾	EX	298-670	(1.2±0.3)(13)	0	1200±150	2	
76 SIM/HEI ²⁾	RN	296	(6.02±1.20)(11)			2	1.2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 HOW/EVE ³)	EX	296	(4.88±0.90)(12)				2
77 SIM/HEI ³)	ES	245-328	7.23(12)	0	705±252		2
78 COX ³)	ES	283	2.47(12)				2
Cl ₂ /H ₂ /NO ₂ photolysis in molar N ₂ /O ₂ . P = 1 atm.							
78 MAR/AND ³)	EX	298	(4.22±1.81)(12)				2
Discharge-flow. Resonance-fluorescence. Unreported T assumed to be 298 K.							
78 PRE ³)	EX	293	(2.4±0.7)(12)				2
Laser Magnetic Resonance Spectrometry.							
78 SIM/HEI ³)	RN	245-328	7.23(12)	0	705±252		2
Determined relative to the reaction: HO ₂ + HO ₂ → H ₂ O ₂ + O ₂ . N ₂ O/H ₂ /O ₂ /NO Photolysis.							
79 BUR/CLI ³)	EX	298	(4.94±1.45)(12)				2
Conventional discharge-flow system.							
79 HOW ³)	EX	232-403	(1.99±0.42)(12)	0	-254±50		2
n = 0 assumed. Discharge-flow. Magnetic-Resonance.							
79 HOW ³)	EX	232-403	(4.79±0.61)(12)	-0.83	0		2
Discharge-flow. Magnetic-Resonance. The preexponential factor expressed as: A(T/298) ^{-0.83} .							
79 LEU ³)	EX	270-425	(3.43±3.37)(12)	0	-130±270		2
Discharge-flow. Resonance-fluorescence.							
80 GLA/LEI ³)	EX	297	(6.63±1.81)(12)				2
Discharge-flow. Same data given in 79 GLA/LEI.							
80 HAC/PRE ³)	EX	293	(4.6±1.0)(12)				2
Isothermal discharge-flow. ESR-LMR Spectrometry.							
80 HOW ³)	EX	232-1271	(2.11±0.21)(12)	0	-240±30		2
Discharge-flow. Laser Magnetic Resonance.							
80 LOR/AZA ³)	EX	873	9.64(11)				2
H ₂ /O ₂ combustion in presence of Propane and NO.							
81 THR/WIL1 ³)	EX	298	(4.16±0.36)(12)				2
Laser magnetic resonance spectrometry.							
³) k _b .							
76 SIM/HEI	RL	295	(9.5±1.5)				2/2
(k _b + k _c)/k _{ref} . Estimated ratio. k _{ref} : HO ₂ + NO ₂ → [HO ₂ NO ₂].							
78 SIM/HEI	RL	245-328	(1.7±0.4)	0	0		2/2
(k _b + k _c)/k _{ref} . k _{ref} : HO ₂ + NO ₂ → HONO + O ₂ (d) → HO ₂ NO ₂ (e)							
T-independent rate ratio assumed. N ₂ O/H ₂ /O ₂ /NO Photolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 COX/DER1 ⁴⁾	ES	296	(8.43±2.11)(10)			2
76 SIM/HEI ⁴⁾ Upper-limit k.	RN	296	<1.20(9)			2
78 SIM/HEI ⁴⁾ N ₂ O/H ₂ /O ₂ /NO photolysis.	ES	245	≈(1.2±0.6)(10)			2
⁴⁾ k _c .						
78 SIM/HEI N ₂ O/H ₂ /O ₂ /NO photolysis. k _c /(k _b + k _c).	RL	245	(3.0±1.0)(-1)			2/2
79 HOW ⁵⁾	EX	271	<1.45(17)			3
79 HOW ⁵⁾	EX	303	<4.72(18)			3
⁵⁾ k _c . M = He + O ₂ . Upper-limit k's. Discharge-flow.						
DO₂ + NO → OD + NO₂						
Hydroperoxo-d + Nitrogen oxide (NO)						
80 GLA/LEI Discharge-flow. Same data given in 79 GLA/LEI.	EX	297	(6.63±2.11)(12)			2
HO₂ + NO₂ (+ M) → HONO + O₂ (+ M) (a) → HO₂NO₂ (+ M) (b)						
Hydroperoxo + Nitrogen oxide (NO ₂)						
75 GLA/TRO ¹⁾ Estimated ratio. k _{ref} : HO ₂ + NO → HO + NO ₂ .	RL	1350-1700	(2.2±0.8)(-1)			2/2
77 LEV/USE ¹⁾ Estimated ratio. k _{ref} : HO ₂ + NO → OH + NO ₂ .	RL	297	(4.3±2.0)(-2)			2/2
78 SIM/HEI ¹⁾ Upper-limit ratio. N ₂ O/H ₂ /O ₂ /NO photolysis. k _{ref} : HO ₂ + NO → OH + NO ₂ (a) → HONO ₂ (b)	RL	245	<8.7(-3)			2/2
¹⁾ k _a /k _{ref} .						
77 LEV/USE k _a /k _b . Estimated ratio.	RL	297	(7.0±0.4)(-1)			2/2
74 SIM/HEI ² ²⁾ Lower-limit k.	ES	298	>1.81(11)			2
75 COX ²⁾	RN	300	(7.23±1.81)(10)			2
75 COX/DER1 ²⁾	ES	296	(7.23±1.81)(10)			2
77 HOW ²⁾ Upper-limit k.	EX	300	<1.81(9)			2
80 LIT ²⁾ Conventional IR Absorption Spectroscopy. P = 30 torr. Upper-limit k.	EX	263	<3.01(10)			2
²⁾ k _a .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 SIM/HEI $k_a + k_b$.	ES	296	(1.18±0.42)(11)			2	
77 COX/DER ³⁾ HONO Photolysis in presence of CO. $k_{ref}: HO_2 + NO \rightarrow OH + NO_2$	RL	273-328	(2.2±0.3)			2/2	
77 LEV/USE ³⁾ $k_{ref}: HO_2 + NO \rightarrow OH + NO_2$. Estimated ratio.	RL	297	(5.8±2.0)(-2)			2/2	
77 SIM/HEI ³⁾ $k_{ref}: HO_2 + NO \rightarrow OH + NO_2$.	RL	245	(6.1±1.5)(-1)			2/2	
78 SIM/HEI ³⁾ $N_2O/H_2/O_2/NO$ photolysis. Estimated ratio. $k_{ref}: HO_2 + NO \rightarrow OH + NO_2$ (a) $\rightarrow HONO_2$ (b)	RL	245	(6.1±1.5)(-1)			2/2	
³⁾ k_b/k_{ref} .							
76 SIM/HEI ⁴⁾	ES	296	(5.90±2.10)(10)			2	
77 SIM/HEI ⁴⁾	ES	245-328	2.53(11)	0	0	2	
78 COX ⁴⁾ High-pressure k, estimated by extrapolation experimental data. $Cl_2/H_2/NO_2$ photolysis in equimolar N_2/O_2 at P = 1 atm.	ES	283	5.42(11)			2	
78 SIM/HEI ⁴⁾ $N_2O/H_2/O_2/NO$ photolysis. T-independent k.	EX	245-328	2.53(11)	0	0	2	
79 COX/PAT ⁴⁾ Limiting high-pressure k. Molecular modulation-UV Absorption spectrometry.	EX	283	(9.03±3.01)(11)			2	
81 MOR/HEI ⁴⁾ Photolysis of NO_2 in presence of HCHO and O_2 , at 360 nm. M = O_2 (54 torr.) + HCHO(2 torr.)	EX	296	4.22(11)			2	2.0
77 HOW ⁴⁾ M = N_2 . M-efficiencies relative to N_2 are: 1.00(N_2), 0.47(He), 0.72(O_2), 3.16(NO_2).	EX	300	(7.58±1.89)(16)			3	
78 COX ⁴⁾ M = $N_2 + O_2$. Low-pressure k, determined on the basis of a simple Lindemann-Hinshelwood model. $Cl_2/H_2/NO_2$ photolysis in equimolar N_2/O_2 . P = 1 atm.	EX	338	(9.07±1.09)(16)			3	
79 COX/PAT ⁴⁾ Limiting low-pressure k. M = $N_2 + O_2$. Molecular modulation-UV Absorption Spectrometry.	EX	283	(9.07±1.81)(16)			3	
⁴⁾ k_b .							


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{HO}_2 + \text{N}_2\text{O} \rightarrow \text{OH} + \text{N}_2 + \text{O}_2$ (a) → any other products (b) Hydroperoxo + Nitrogen oxide (N_2O)						
79 HOW k_a . Discharge-flow system. Laser Magnetic Resonance. Upper-limit k.	EX	300-394	<3.01(6)			2
79 GRA/WIN k_{overall} . Thermolysis of HO_2NO_2 . Upper-limit k. P(Total) = 760 torr.	EX	300	≤1.20(4)			2
79 HOW k_{overall} . Discharge-flow system. Laser Magnetic Resonance. Upper-limit k.	EX	300-394	≤3.0(7)			2
$\text{HO}_2 + \text{NH}_2 \rightarrow \text{NH}_3 + \text{O}_2$ (a) → $\text{H}_2\text{O} + \text{HNO}$ (b) Hydroperoxo + Amidogen						
79 CHE/SAR $k_a + k_b$. NH_3 flash-photolysis. Laser Spectroscopy. P = (100-570) torr.	EX	298	(1.51±0.30)(13)			2
79 LOZ/NAD $k_a + k_b$. Intracavity Laser Spectroscopy. Flash-photolysis. P = (10-760) torr.	RN	298	(3.67±1.51)(13)			2
79 NAD/SAR1 $k_b/(k_a + k_b)$. NH_3/O_2 Pulse-photolysis. Intracavity Laser Spectroscopy. Lower-limit ratio.	RL	298	≥3.0(-1)			2/2
$\text{HO}_2 + \text{CO} (+ \text{M}) \rightarrow \text{OH} + \text{CO}_2 (+ \text{M})$ Hydroperoxo + Carbon monoxide						
72 VAR/DAN	EX	878-952	1.33(14)	0	11575±1510	2
72 WES/DEH1 k_{ref} : $\text{HO}_2 + \text{H} \rightarrow \text{OH} + \text{OH}$. Estimated ratio.	RL	298	(6.0±2.0)(-2)			2/2
73 GOR Upper-limit k.	EX	298	<9.6(7)			2
73 DAV/PAY Estimated, upper-limit k.	ES	300	≤6.02(3)			2
73 SIM/HEI1 Estimated, upper-limit k.	ES	373-473	<3.01(6)			2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 WYR/WEN Upper limit k derived from spectroscopic observations.	EX	310	≤1.6(10)			2
74 WYR/WEN Upper limit k derived from CO ₂ yield measurements.	EX	310	≤2.0(6)			2
75 VAR/SAC	EX	878-952	(1.07±0.30)(14)	0	11575±1510	2
77 ATR/BAL P(Total) = 500 torr. Determined relative to the reaction: HO ₂ + HO ₂ → H ₂ O ₂ + O ₂ .	RN	~773	5.8(13)	0	11547	2
77 COL/NAE	ES	1110	5.6(9)			2 4.0
79 BUR/CLI Discharge-flow. Upper-limit k.	EX	298	≤1.20(7)			2
79 GRA/WIN Thermolysis of HO ₂ NO ₂ . Upper-limit k. P(Total) = 760 torr.	EX	300	≤1.20(5)			2
79 HOW ¹⁾	EX	304	<2.41(7)			2
79 HOW ¹⁾	EX	394	<3.61(9)			2
¹⁾ Discharge-flow. Upper-limit k's.						
79 BUR/CLI M = He. Discharge-flow. Upper-limit k.	EX	298	≤1.45(14)			3
HO ₂ + CH ₄ → H ₂ O ₂ + CH ₃ Hydroperoxo + Methane						
72 SKI/LIF	ES	1000-2500	2.0(13)	0	9059	2
HO ₂ + HCCHO → O ₂ + CH ₂ OH (a) → H ₂ O ₂ + CHO (b) → HO ₂ CH ₂ O → HOCH ₂ O ₂ (c) Hydroperoxo + Formaldehyde						
81 TSU/HAS k _a . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ in Ar behind reflected shock-waves. k ₁ = k ₋₁ K.	DE	1200-1800	3.39(12)	0	9623	2
71 BAL/LAN ¹⁾	ES	713	1.36(9)			2
71 BAL/LAN ¹⁾	ES	673-773	1.0(12)	0	5033±1007	2
72 BAL/FUL ¹⁾	DE	673-773	9.6(8)			2
71 VAR/SAC ¹⁾ Oxidation in quartz reactor.	EX	773-973	1.14(13)	0	5234±1510	2
¹⁾ k _b .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 SU/CAL3 k _c . Photolysis of Cl ₂ /HCHO mixtures diluted in synthetic air. FTIR Spectroscopy. P(Total) ~ 700 torr.	ES	298	~6.02(9)			2
82 VEY/RAY k _c . HCHO/O ₂ /NO flash-photolysis. Data-fit by computer simulation on the basis of a proposed mechanism. [NO] ₀ = (15-200) torr. [O ₂] ₀ = (2.5-45) torr. [HCHO] ₀ = (2-30) torr.	DE	298	(4.52±2.11)(10)			2
HO₂ + CH₃O₂ → O₂ + CH₃OOH						
Hydroperoxo + Methylendioxy						
79 COX/TYN ¹)	EX	274	(5.12±0.72)(12)			2
79 COX/TYN ¹)	EX	298	(3.61±0.54)(12)			2
79 COX/TYN ¹)	EX	338	(2.11±0.30)(12)			2
80 COX/TYN ¹) P = 760 torr.	EX	275-338	4.63(10)	0	-1296±364	2 3.4
¹) Molecular Modulation UV-Absorption Spectrometry.						
HO₂ + CH₃OH → H₂O₂ + CH₂OH						
Hydroperoxo + Methanol						
81 TSU/HAS M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures mixtures diluted in Ar, behind reflected shock-waves.	ES	1200-1800	1.0(12)	0	5052	2
HO₂ + CH₂=CH₂ → OH + 						
Hydroperoxo + Ethene						
73 WAL2 k _{ref} :	RL	773	(1.6±0.2)(-2)			2/2
HO ₂ + HCHO → H ₂ O ₂ + CHO						
73 WAL2	ES	773	1.5(7)			2
81 BAL/WAL1 Oxidation of Ethene in H ₂ /O ₂ mixtures in aged boric-acid-coated vessels.	ES	773	(5.0±1.0)(7)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
HO₂ + CH₃CH₃ → H₂O₂ + CH₃CH₂						
Hydroperoxo + Ethane						
71 BAL/LAN k _{ref} : CH ₃ CH ₃ + HCHO → products. Estimated ratio.	RL	713	2.8(-2)			2/2
73 BAL/FUL k _{ref} : HO ₂ + HCHO → H ₂ O ₂ + CHO. Rate ratio per primary C-H bond: k _{prim} /k _{ref} = 0.005	RL	773	3.0(-2)			2/2
73 BAL/FUL Rate constant per primary C-H bond: k _{prim} = 5.1x10 ⁶ cm ³ mol ⁻¹ s ⁻¹	RN	773	3.06(7)			2
HO₂ + CH₃CHO → H₂O₂ + CH₃CO						
Hydroperoxo + Acetaldehyde						
77 COL/NAE	ES	1030-1115	1.70(12)	0	5350	2 4.0
HO₂ + CH₂CH₂OH → O₂ + CH₃CH₂OH (a) → H₂O + HCHO + HCHO (b)						
Hydroperoxo + Ethyl, 2-hydroxy-						
76 MEA/HEI k _a /k _b .	RL	298	1.2			2/2
HO₂ + CH₃CH=CH₂ → OH + 						
Hydroperoxo + 1-Propene						
77 SAR/VAR Oxidation of Formaldehyde in presence of Propane. Upper-limit k.	ES	823	≤1.08(8)			2
81 BAL/WAL1 Oxidation of 1-Propene in H ₂ /O ₂ mixtures, in aged boric-acid- coated vessels.	ES	773	1.5(8)			2
HO₂ + CH₃CH₂CH₃ → H₂O₂ + (CH₃)₂CH (a) → H₂O₂ + CH₃CH₂CH₂ (b)						
Hydroperoxo + Propane						
71 BAL/LAN (k _a + k _b)/k _{ref} . k _{ref} : HCHO + CH ₃ CH ₂ CH ₃ → products.	RL	713	7.8(-2)			2/2
71 BAL/LAN k _a + k _b .	RL	713	7.86(7)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 BAL/FUL k_a/k_{ref} . k_{ref} : $HO_2 + HCHO \rightarrow H_2O_2 + CHO$. Rate ratio per secondary C-H bond: $k_{sec}/k_{ref} = 0.024$	RL	773	4.8(-2)			2/2
73 BAL/FUL k_a . Rate constant per secondary C-H bond: $k_{sec} = 2.4 \times 10^7 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	RN	773	4.8(7)			2
73 BAL/FUL k_b/k_{ref} . k_{ref} : $HO_2 + HCHO \rightarrow H_2O_2 + CHO$. Rate ratio per primary C-H bond: $k_{prim}/k_{ref} = 0.005$	RL	773	3.0(-2)			2/2
73 BAL/FUL k_b . Rate constant per primary C-H bond: $k_{prim} = 5.1 \times 10^6 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	RN	773	3.06(7)			2
$HO_2 + CH_3CH_2CHO \rightarrow H_2O_2 + CH_3CH_2CO$ Hydroperoxo + Propanal						
71 BAL/LAN	ES	713	1.82(9)			2
79 BAL/LEW1 Oxidation in an aged boric-acid-coated-vessel.	RN	713	(1.52±0.15)(9)			2
$HO_2 + \text{trans-}CH_3CH=CHCH_3 \rightarrow \text{products}$ Hydroperoxo + 2-Butene, (E)-						
79 GRA/WIN Thermolysis of HO_2NO_2 . Upper-limit k. P(Total) = 760 torr.	EX	300	≤2.41(6)			2
$HO_2 + (CH_3)_3CH \rightarrow H_2O_2 + (CH_3)_3C$ (a) $\rightarrow H_2O_2 + (CH_3)_2CHCH_2$ (b) Hydroperoxo + Propane, 2-methyl-						
73 BAL/FUL k_a/k_{ref} . k_{ref} : $HO_2 + HCHO \rightarrow H_2O_2 + CHO$. Rate ratio per tertiary C-H bond: $k_{tert}/k_{ref} = 0.133$	RL	773	1.33(-1)			2/2
73 BAL/FUL k_a . Rate constant per tertiary C-H bond: $k_{tert} = 1.4 \times 10^8 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	RN	773	1.35(8)			2
73 BAL/FUL k_b/k_{ref} . k_{ref} : $HO_2 + HCHO \rightarrow H_2O_2 + CHO$. Rate ratio per primary C-H bond: $k_{prim}/k_{ref} = 0.005$	RL	773	4.5(-2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 BAL/FUL k_b . Rate constant per primary C-H bond: $k_{\text{prim}} = 5.1 \times 10^6 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	RN	773	4.59(7)			2
71 BAL/LAN $(k_a + k_b)/k_{\text{ref}}$. k_{ref} : $\text{HCHO} + (\text{CH}_3)_3\text{CH} \rightarrow \text{products}$.	RL	713	1.55(-1)			2/2
73 BAL/FUL $(k_a + k_b)/k_{\text{ref}}$.	RL	773	1.78(-1)			2/2
73 BAL/FUL $k_a + k_b$.	RN	773	1.81(8)			2
$\text{HO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} \rightarrow \text{H}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CO}$ Hydroperoxo + Butanal						
71 BAL/LAN	ES	713	2.41(9)			2
$\text{HO}_2 + (\text{CH}_3)_2\text{CHCHO} \rightarrow \text{H}_2\text{O}_2 + (\text{CH}_3)_2\text{CHCO}$ (a) $\rightarrow \text{H}_2\text{O}_2 + (\text{CH}_3)_2\text{CCHO}$ (b) $\rightarrow \text{H}_2\text{O}_2 + \text{CH}_2\text{CH}(\text{CH}_3)\text{CHO}$ (c)						
Hydroperoxo + Propanal, 2-methyl-						
79 BAL/CLE ¹⁾ k_a .	EX	713	(1.83±0.10)(9)			2
79 BAL/CLE ¹⁾ k_b .	EX	713	(1.4±0.2)(8)			2
¹⁾ Oxidation in an aged boric-acid-coated vessel. P(Total) = 60 Atm.						
$\text{HO}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{products}$ Hydroperoxo + 2-Butene, 2,3-dimethyl-						
79 GRA/WIN Thermolysis of HO_2NO_2 . Upper-limit k. P(Total) = 760 torr.	EX	300	≤2.41(7)			2
$\text{HO}_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{H}_2\text{O}_2 + (\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2$ Hydroperoxo + Butane, 2,3-dimethyl-						
75 ALC/MIL Optimization.	ES	373	2.5(5)			2
77 ALC/MIL Azomethane photolysis. Optimization.	ES	373	2.5(5)			2
$\text{H}_2\text{O} (+ \text{M}) \rightarrow \text{H} + \text{OH} (+ \text{M})$ Water						
78 BOP/KER Shock-tube system. M = Ar/Kr mixture.	EX	3600-4800	1.26(14)	0	50327±1510	2 1.6

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
D₂O (+ M) → D + OD (+ M)							
Water-d ₂							
78 BOP/KER Shock-tube system. M = Ar/Kr mixture.	EX	3600-4800	1.26(14)	0	50327±1510	2	1.6
H₂O + SO₃ → H₂SO₄							
Water + Sulfur trioxide							
75 CAS/DAV	EX	298	(5.48±1.20)(11)			2	
H₂O + NO₂ → OH + HONO							
Water + Nitrogen oxide (NO ₂)							
76 FIF k ₁ = k ₋₁ K.	DE	1000-1380	8.3(12)	0	21138	2	
H₂O + NO₂ + NO₂ → HONO + HONO₂							
Water + Nitrogen oxide (NO ₂)							
74 ENG/COR	EX	298	(5.50±0.29)(10)			3	
74 ENG/COR A and B recalculated from the reported data.	EX	298-323	(7.79±1.09)(9)	0	-580±43	3	1.1
79 STR/WEL Tunable diode-laser. Static reactor. Based on k ₁ = k ₋₁ K and thermochemical data.	DE	296	2.90(9)			3	
H₂O + N₂O₃ → HNO₂ + HNO₂							
Water + Nitrogen oxide (N ₂ O ₃)							
75 ENG/COR	RN	298	1.2(7)			2	
75 ENG/COR A and B recalculated from the reported data.	RN	313-323	(5.88±2.24)(13)	0	4605±120	2	
H₂O + N₂O₄ → HONO + HONO₂							
Water + Nitrogen oxide (N ₂ O ₄)							
74 ENG/COR	EX	298	8.12(5)			2	
74 ENG/COR A and B recalculated from the reported data.	EX	298-323	(3.74±0.76)(14)	0	5954±64	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
H₂O + N₂O₅ → HONO₂ + HONO₂						
Water + Nitrogen oxide (N ₂ O ₅)						
73 MOR/NIK2 Upper-limit k.	EX	298	≤7.83(3)			2
H₂O₂ (+ M) → OH + OH (+ M) (a) → any other products (b)						
Hydrogen peroxide						
71 KIJ/TRO k _a . M = Ar. Shock waves.	EX	870-1400	1.58(16)	0	21641	2
79 BAS/KOG k _a . M = Ar. Flow-reactor.	EX	1095-1253	4.07(16)	0	21137±1761	2 4.5
71 TES/FOR	EX	717-754	3.16(18)	0	23553±654	2 2.51
H₂O₂ + NO → OH + HONO						
Hydrogen peroxide + Nitrogen oxide (NO)						
72 GRA/LIS Upper-limit k. The reaction is assumed to occur entirely in gas phase.	EX	298	≤3.10(14)			2
80 LIT IR-Absorption Spectroscopy. Upper-limit k. The reaction might be heterogeneous.	EX	263-283	≤6.02(4)			2
H₂O₂ + NO₂ → HONO₂ + 1/2H₂O + 1/4O₂ (overall)						
Hydrogen peroxide + Nitrogen oxide (NO ₂)						
72 GRA/LIS Upper-limit k.	ES	298	≤6.0(5)			2
H₂O₂ + N₂O₅ → HOONO₂ + HONO₂						
Hydrogen peroxide + Nitrogen oxide (N ₂ O ₅)						
80 LIT IR-Absorption Spectroscopy. Upper limit k. P = (10-80) torr.	EX	253-283	<6.02(5)			2
H₂O₂ + HONO₂ → products						
Hydrogen peroxide + Nitric acid						
80 LIT IR-Absorption Spectroscopy. Upper-limit k.	EX	263-283	<6.02(4)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
S + O₂ → SO + O						
Sulfur atom + Oxygen molecule						
71 FAI/VAN Flash photolysis. Vacuum-UV Kinetic Spectroscopy.	EX	298	(1.7±0.2)(12)			2
72 DAV/KLE1	EX	252-423	(1.35±0.16)(12)	0	0±50	2
72 DON/LIT	EX	295	(1.0±0.2)(12)			2
75 CLY/TOW	EX	298	(9.03±1.87)(11)			2
79 CLY/WHI Resonance-fluorescence. Microwave-discharge.	EX	296-410	(1.02±0.30)(12)	0	-153±108	2
S + O₃ → SO + O₂						
Sulfur atom + Ozone						
75 CLY/TOW	EX	298	(7.23±1.87)(12)			2
S(¹D) + H₂ → products						
Sulfur atom + Hydrogen molecule						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	2.2(-1)			2
S + S (+ M) → S₂ (+ M)						
Sulfur atom						
79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum. Computer simulation. P = (0.1-2) torr.	DE	295	(4.3±0.6)(18)			3
S + SH → S₂ + H						
Sulfur atom + Mercapto						
79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum. Computer simulation. P = (0.1-2) torr. Upper-limit k.	DE	295	<3.0(12)			2
S(¹D) + N₂ → products						
Sulfur atom + Nitrogen molecule						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	6.2(-2)			2/2
S(¹D) + NO → products						
Sulfur atom + Nitrogen oxide (NO)						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	6.8(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
S + NO (+ M) → SNO (+ M)						
Sulfur atom + Nitrogen oxide (NO)						
78 VAN/OBI ¹⁾ M = CO ₂ . Low-pressure k. P(CO ₂) <100 torr.	EX	298	(1.9±0.1)(17)			3
78 VAN/OBI ¹⁾ M = CO ₂ . Limiting high-pressure k.	EX	298	(9.3±2.1)(12)			2
¹⁾ Flash-photolysis. Vacuum-UV Absorption Spectroscopy.						
S + NO₂ → SO + NO						
Sulfur atom + Nitrogen oxide (NO ₂)						
75 CLY/TOW	EX	298	(3.73±0.85)(13)			2
79 CLY/WHI Resonance-fluorescence. Microwave-discharge.	EX	296-410	(2.95±0.60)(13)	0	-84±60	2
S(¹D) + N₂O → NS + NO						
Sulfur atom + Nitrogen oxide (N ₂ O)						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	≈1.0(-1)			2/2
S(¹D) + CO → products						
Sulfur atom + Carbon monoxide						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	1.9(-1)			2/2
S(¹D) + CO₂ → products						
Sulfur atom + Carbon dioxide						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	2.4(-1)			2/2
S(¹D) + CH₄ → CH₃SH						
Sulfur atom + Methane						
72 LIT/DAL k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.	RL	300	7.6(-2)			2/2
80 ADD/DON CS ₂ photolysis. Time-Resolved Resonance-fluorescence.	EX	295	(1.08±0.18)(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
S + COS → S₂ + CO						
Sulfur atom + Carbon oxide sulfide						
72 JAK/AHM	RL	298	8.3(1)			2/2
k _{ref} : S + CH ₂ =CH ₂ → \underline{S}						
72 JAK/AHM	RN	298	1.1(10)			2
74 KLE/DAV	EX	233-445	(9.15±1.20)(11)	0	1827±60	2
S(¹D) + COS → S₂ + CO						
Sulfur atom + Carbon oxide sulfide						
72 LIT/DAL	RL	300	(1.5±0.5)			2/2
k _{ref} : S(¹ D) + CH ₂ =CH ₂ → products.						
79 ADD/BYR	EX	290	(7.23±1.81)(13)			2
COS UV-photolysis. Time-Resolved Atomic Absorption Spectroscopy.						
79 SHE/SAF ¹⁾	RL	298	2.4			2/2
k _{ref} : S(¹ D) + COS → S + COS.						
79 SHE/SAF ¹⁾	RL	298	5.7(-1)			2/2
k _{ref} : S(¹ D) + CH ₂ =CH ₂ → CH ₂ =CHSH (a)						
→ \underline{S}^{\dagger} (b)						
(k _{ref} = k _a + k _b .)						
¹⁾ UV-photolysis of COS in a high-vacuum system. Optimization.						
80 ADD/DON	EX	295	(1.81±0.60)(14)			2
CS ₂ photolysis. Time-Resolved Resonance-Fluorescence.						
S + CH=CH → \underline{S} (a)						
→ :CHCHS [†] (b)						
Sulfur atom + Ethyne						
71 STR/O'C	RL	298-450	6.2	0	1007	2/2
k _a /k _{ref} . Conventional photolysis method.						
k _{ref} : S + CH ₂ =CH ₂ → \underline{S}						








4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 LIT/DON k _a . Flash-photolysis of COS in Ar. P(COS) = 0.1 torr. P(Ar) = 150 torr.	EX	295	(3.01±0.30)(11)			2
78 VAN/SAF ¹⁾	EX	298	(2.3±0.4)(11)			2
78 VAN/SAF ¹⁾	EX	298-484	(3.4±1.9)(13)	0	1510±201	2
¹⁾ k _b . Flash-photolysis. Vacuum-UV Absorption Spectroscopy. A spin-allowed, least motion primary path is assumed.						
S(¹D) + CH=CH → Δ^{\ddagger}						
Sulfur atom + Ethyne						
73 LIT/DON COS Flash-photolysis in Ar. k _{ref} : S(¹ D) + CO ₂ → S(³ P) + CO ₂ . P(Ar) = 150 torr.	RL	295	(2.5±0.4)			2/2
S + CD=CD → :CDCDS[†]						
Sulfur atom + Ethyne-d ₂						
78 VAN/SAF Flash-photolysis. Vacuum-UV Absorption Spectroscopy. A spin-allowed, least motion primary path is assumed.	EX	298	(2.3±0.4)(11)			2
S + CH₂=CH₂ → Δ^{\ddagger}						
Sulfur atom + Ethene						
71 CON/VAN Flash-photolysis method.	EX	298	(9.0±1.0)(11)			2
71 STR/O'C Conventional photolysis method.	ES	298-450	≤1.0(13)	0	755	2
72 DAV/KLE2	ES	218-442	(4.29±0.45)(12)	0	795±40	2
S + CH₂=CD₂ → $\Delta^{\ddagger}_{D_2}$						
Sulfur atom + Ethene-1,1-d ₂						
71 STR/O'C Conventional photolysis method. k _{ref} : S + CH ₂ =CH ₂ → Δ^{\ddagger}	RL	298-450	1.07	0	0	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + \text{cis-CHD=CHD} \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{D} \quad \text{D} \end{array}$						
Sulfur atom + Ethene-1,2-d ₂ , (Z)- 71 STR/O'C Conventional photolysis method.	RL	298-450	1.04	0	0	2/2
$k_{\text{ref}}: S + \text{CH}_2=\text{CH}_2 \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{H} \end{array}$						
$S + \text{CD}_2=\text{CD}_2 \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{D} \quad \text{D} \end{array}$						
Sulfur atom + Ethene-d ₄ 71 STR/O'C Conventional photolysis method.	RL	298-450	1.14	0	0	2/2
$k_{\text{ref}}: S + \text{CH}_2=\text{CH}_2 \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{H} \end{array}$						
$S(^1D) + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHSH} \quad (\text{a})$ $\rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{H} \end{array} \quad (\text{b})$						
Sulfur atom + Ethene 79 SHE/SAF 1) k_a	RN	298	4.2(13)			2
79 SHE/SAF 1) k_b	DE	298	3.8(13)			2
1) UV-photolysis of COS. Optimization.						
$S(^1D) + \text{CH}_3\text{CH}_3 \rightarrow \text{products}$						
Sulfur atom + Ethane 72 LIT/DAL	RL	300	1.7(-1)			2/2
$k_{\text{ref}}: S(^1D) + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHSH} \quad (\text{a})$ $\rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{H} \end{array} \quad (\text{b})$						
$S + \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{H} \end{array} \rightarrow \text{S}_2 + \text{CH}_2=\text{CH}_2$						
Sulfur atom + Thiirane (Ethylene episulfide) 71 STR/O'C Conventional photolysis method.	RL	298-450	8.3	0	-906	2/2
$k_{\text{ref}}: S + \text{CH}_2=\text{CH}_2 \rightarrow \begin{array}{c} \text{S} \\ \diagup \quad \diagdown \\ \text{H} \quad \text{H} \end{array}$						

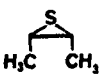

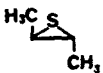





4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + CH_3C\equiv CH \rightarrow$  (a)						
$\rightarrow :C(CH_3)CHS^\ddagger$ (b)						
Sulfur atom + 1-Propyne						
71 STR/O'C	RL	298-450	6.2	0	453	2/2
k_a/k_{ref} . Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow$ 						
78 VAN/SAF ¹⁾	EX	298	(4.8±0.2)(12)			2
78 VAN/SAF ¹⁾	EX	298-449	(2.0±1.2)(13)	0	453±101	2
¹⁾ k_p . Flash-photolysis.						
Absorption spectroscopy. A spin-allowed, least motion primary path assumed.						
$S + CH_3CH=CH_2 \rightarrow$ 						
Sulfur atom + 1-Propene						
71 CON/VAN ¹⁾	RL	298	(7.5±1.3)			2/2
$k_{ref}: S + CH_2=CH_2 \rightarrow$ 						
71 CON/VAN ¹⁾	RN	298	(6.0±1.0)(11)			2
¹⁾ Flash-photolysis.						
71 STR/O'C	RL	298-450	1.0	0	-574	2/2
Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow$ 						
73 KLE/DAV2	EX	214-500	(3.63±0.43)(12)	0	191±45	2
$S +$  $\rightarrow S_2 + CH_3CH=CH_2$						
Sulfur atom + Thiirane, methyl-						
71 STR/O'C	RL	298-450	8.4	0	-1057	2/2
Conventional photolysis.						
$k_{ref}: S + CH_2=CH_2 \rightarrow$ 						
$S + CH_3CH_2C\equiv CH \rightarrow :C(CH_2CH_3)CHS^\ddagger$						
Sulfur atom + 1-Butyne						
78 VAN/SAF	EX	298	(3.3±0.2)(12)			2
Flash-photolysis.						
Absorption Spectroscopy. A spin allowed, least motion primary path assumed.						



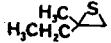
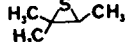
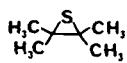
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + CH_3C\equiv CCH_3 \rightarrow H_3C-\overset{\triangle S}{C}-CH_3$ (a) $\rightarrow :C(CH_3)C(S)CH_3 \uparrow$ (b) Sulfur atom + 2-Butyne	71 STR/O'C	RL 298-450	2.7	0	-654	2/2
k_a/k_{ref} Conventional photolysis. k_{ref} : $S + CH_2=CH_2 \rightarrow \overset{\triangle S}{C}$						
78 VAN/SAF k_b . Flash-photolysis. Absorption-spectroscopy. A spin-allowed, least motion primary path assumed.	EX 298		(1.6±0.2)(13)			2
$S + CH_2=CHCH=CH_2 \rightarrow H_2C=HC-\overset{\triangle S}{C}$ Sulfur atom + 1,3-Butadiene	71 STR/O'C	RL 298-450	2.4	0	-1027	2/2
Conventional photolysis. k_{ref} : $S + CH_2=CH_2 \rightarrow \overset{\triangle S}{C}$						
$S + CH_3CH_2CH=CH_2 \rightarrow H_3CCH_2-\overset{\triangle S}{C}$ Sulfur atom + 1-Butene	71 CON/VAN ¹⁾	RL 298	(1.1±0.2)(1)			2/2
k_{ref} : $S + CH_2=CH_2 \rightarrow \overset{\triangle S}{C}$						
71 CON/VAN ¹⁾ ¹⁾ Flash-photolysis method.	RN 298		(9.1±1.0)(12)			2
71 STR/O'C Conventional photolysis. k_{ref} :	RL 298-450		7.5(-1)	0	-866	2/2
$S + CH_2=CH_2 \rightarrow \overset{\triangle S}{C}$						
73 KLE/DAV2	EX 216-475		(4.46±0.69)(12)	0	181±45	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + \text{cis-CH}_3\text{CH=CHCH}_3 \rightarrow$ 						
Sulfur atom + 2-Butene, (Z)- 71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298-450	5.3(-1)	0	-1052	2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$ 						
73 DAV/KLE	EX	219-500	(2.82±0.42)(12)	0	-116±45	2
$S + \text{trans-CH}_3\text{CH=CHCH}_3 \rightarrow$ 						
Sulfur atom + 2-Butene, (E)- 71 CON/VAN ¹⁾ $k_{\text{ref}}:$	RL	298	(1.5±0.3)(1)			2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$ 						
71 CON/VAN ¹⁾	RN	298	(1.2±0.2)(13)			2
¹⁾ Flash-photolysis method.						
71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298-450	6.5(-1)	0	-1012	2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$ 						
$S + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow$ 						
Sulfur atom + 1-Propene, 2-methyl- 71 CON/VAN ¹⁾ $k_{\text{ref}}:$	RL	298	(4.5±0.6)(1)			2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$ 						
71 CON/VAN ¹⁾	RN	298	(3.6±0.5)(13)			2
¹⁾ Flash-photolysis.						
71 STR/O'C Conventional photolysis. $k_{\text{ref}}:$	RL	298-450	9.7(-1)	0	-1188	2/2
$S + \text{CH}_2=\text{CH}_2 \rightarrow$ 						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$S + CH_3CH_2C=CH_3 \rightarrow :C(CH_3)C(S)CH_2CH_3^\ddagger$ (a) $\rightarrow :C(CH_2CH_3)C(S)CH_3^\ddagger$ (b)						
Sulfur atom + 2-Pentyne						
78 VAN/SAF	EX	298	(1.8±0.2)(13)			2
$k_a + k_b$. Flash-photolysis. Absorption Spectroscopy. A spin-allowed, least motion primary path assumed.						
$S + $  $\rightarrow $ 						
Sulfur atom + Cyclopentene						
71 STR/O'C	RL	298-450	6.7(-1)	0	-1082	2/2
Conventional photolysis. $k_{ref}: S + CH_2=CH_2 \rightarrow \triangle S$						
$S + CH_3CH_2C(CH_3)=CH_2 \rightarrow $ 						
Sulfur atom + 1-Butene, 2-methyl-						
71 STR/O'C	RL	298-450	7.8(-1)	0	-1424	2/2
Conventional photolysis. $k_{ref}: S + CH_2=CH_2 \rightarrow \triangle S$						
$S + (CH_3)_2C=CHCH_3 \rightarrow $ 						
Sulfur atom + 2-Butene, 2-methyl-						
71 STR/O'C	RL	298-450	5.1(-1)	0	-1515	2/2
Conventional photolysis. $k_{ref}: S + CH_2=CH_2 \rightarrow \triangle S$						
$S + (CH_3)_2C=C(CH_3)_2 \rightarrow $ 						
Sulfur atom + 2-Butene, 2,3-dimethyl-						
71 CON/VAN ¹)	RL	298	(7.7±1.0)(1)			2/2
$k_{ref}: S + CH_2=CH_2 \rightarrow \triangle S$						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 CON/VAN ¹⁾ Lower-limit k.	RN	298	≥(6.2±0.8)(13)			2	
¹⁾ Flash-photolysis.							
71 STR/O'C Conventional photolysis.	RL	298-450	5.0(-1)	0	-1691	2/2	
$k_{\text{ref}}: \text{S} + \text{CH}_2=\text{CH}_2 \rightarrow \text{S}$							
73 DAV/KLE	EX	252-500	(2.82±1.02)(12)	0	-649±116	2	
S₂ (+ M) → S + S (+ M)							
Sulfur dimer							
80 HIG/SAI M = Ar. COS pyrolysis behind incident shock-waves. Possibly an upper-limit k. P = (240-380) torr.	EX	4500-6000	4.79(13)	0	38752	2	
S₂ + S₂ (+ M) → S₄ (+ M)							
Sulfur dimer							
72 LAN/OLD M = CO ₂ .	ES	293	9.07(17)			3	10.0
73 LAN/OLD M = CO ₂ .	ES	293	3.6(18)			3	5.0
79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum. k determined by computer simulation. P = (0.1-2) torr.	DE	295	(8.0±1.0)(18)			3	
SO (+ M) → S + O (+ M)							
Sulfur monoxide							
78 AST/GLA M = Ar. Incident or reflected shock-waves. Rate constant expressed as k[Ar].	EX	5700-7200	1.58(14)	0	55331±3608	2	4.0
SO + O₂ → SO₂ + O							
Sulfur monoxide + Oxygen molecule							
72 BRE/MIL Fast-flow. EPR detection. Upper-limit k. P(Total) = 0.45 torr.	EX	297	<5.0(7)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 BLA/SHA1 ¹⁾	EX	298	(6.44±0.96)(7)			2	
82 BLA/SHA2 ¹⁾	EX	230-420	1.44(11)	0	2370±250	2	2.1
¹⁾ ArF Laser-photodissociation of SO ₂ at 193 nm. in He. P(He) < 400 torr. P(SO ₂) ~ 30 mtorr. P(O ₂) < 500 torr.							
SO + SO (+ M) → SO₂ + S (+ M)							
Sulfur monoxide							
72 BRE/MIL Fast-flow technique with EPR detection. P(Total) = 0.45 torr. Upper-limit k.	EX	297	<3.0(10)			2	
75 CHU/CAL Best fit.	ES	298	(5.0±4.0)(8)			2	
80 HER/HUI M = N ₂ . Tubular flow-reactor. Mass-spectrometry.	EX	298	1.6(17)			3	
SO + SO₃ → SO₂ + SO₂							
Sulfur monoxide + Sulfur trioxide							
75 CHU/CAL Best fit.	ES	298	(1.2±0.7)(9)			2	
SO + (SO)₂ → SO₂ + S₂O							
Sulfur monoxide + Sulfur monoxide dimer							
80 HER/HUI Tubular flow-reactor. Mass-spectrometry.	EX	298	2.0(10)			2	
SO + NO₂ → SO₂ + NO							
Sulfur monoxide + Nitrogen oxide (NO ₂)							
71 MIY/TAK2	EX	298	(1.23±0.15)(12)			2	
80 CLY/MAC Discharge-flow. Mass-spectrometry.	EX	295	(8.19±0.60)(12)			2	
82 BLA/SHA1 ArF Laser-photodissociation of SO ₂ at 193 nm. in presence of diluent gas. P(He) = (100-500) torr. P(SO ₂) ~ 30 mtorr.	EX	298	(8.91±1.20)(12)			2	
SO₂ (+ M) → SO + O (+ M)							
Sulfur dioxide							
75 KIE M = Kr. Incident shock-waves. (3-30)% SO ₂ and (70-97)% Kr.	EX	2900-5200	1.70(16)	0	56366±2013	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 AST/GLA M = Ar. Incident or reflected shock-waves. [Ar] = (0.3-4.0)x10 ¹⁹ molec.cm ⁻³ Rate constant expressed as k[Ar].	EX	3700-7500	3.98(14)	0	53888±2165	2	2.0
78 JUS/RIM M = Ar. Reflected shock-waves.	EX	2500-3400	2.9(16)	0	58590±2270	2	2.2
79 GRI/REE ¹⁾ Total dens.: (0.5-2.0)x10 ¹⁹ molec.cm ⁻³ .	EX	2800-3880	(8.0±2.0)(15)	0	54353	2	
79 GRI/REE ¹⁾ Extended T-range, for M = Ar, or Kr. About a factor of 20 above literature values.	SE	2500-5200	1.5(16)	0	56366	2	
¹⁾ M = Ar. Reflected shock-waves.							
80 RAJ/BAB ²⁾ M = Ar.	EX	4000-6000	3.34(15)	0	54152	2	
80 RAJ/BAB ²⁾ M = SO ₂ .	EX	4000-6000	5.02(14)	0	33518	2	
²⁾ Thermolysis of SO ₂ behind incident shock-waves. P = (1.0-2.5) torr.							
80 SAI/YOK2 M = Ar. Thermolysis of SO ₂ behind reflected shock-waves. Total dens. = (0.5-1.4)x10 ¹⁸ molec.cm ⁻³ .	EX	4300-6200	3.55(14)	0	52805	2	
82 RAJ/BAB ³⁾ M = Ar.	EX	4000-6000	3.34(15)	0	54152	2	
82 RAJ/BAB ³⁾ M = SO ₂ .	EX	4000-6000	5.02(14)	0	33518	2	
³⁾ Dissociation of SO ₂ behind incident shock-waves, in Ar. Gas-chromatography. P ₀ = (1.0-2.5) torr.							
SO₂ + SO₂(¹B₁) → SO(¹Δ_g, ³Σ⁻) + SO₃							
Sulfur dioxide							
75 CHU/CAL	ES	298	(2.2±0.5)(12)			2	
SO₂ + SO₂(³B₁) → SO(³E⁻) + SO₃							
Sulfur dioxide							
75 CHU/CAL	ES	298	(4.2±0.4)(10)			2	
SO₂ + NO₂ → SO₃ + NO							
Sulfur dioxide + Nitrogen oxide (NO ₂)							
71 ARM/CUL	EX	703-1193	6.31(12)	0	13588	2	
77 FRE/PAL	EX	703-1850	6.31(12)	0	13588	2	
Extended validity of k reported in 71 ARM/CUL.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
SO₂ + NO₃ → SO₃ + NO₂							
Sulfur dioxide + Nitrogen dioxide (NO ₂)							
75 DAU/CAL Upper-limit k.	ES	300	≤4.2(3)			2	
SO₂ + N₂O₅ → SO₃ + N₂O₄							
Sulfur dioxide + Nitrogen oxide (N ₂ O ₅)							
75 DAU/CAL Upper-limit k.	ES	300	≤2.5(1)			2	
SO₂ + CO → products							
Sulfur dioxide + Carbon monoxide							
71 BAU/JEF M = Ar. P = (27-170) torr.	EX	1770-2453	2.69(12)	0	24303±604	2	1.32
SO₂[*] + CO → SO + CO₂							
Sulfur dioxide + Carbon monoxide							
73 CEH/HEI ¹⁾ At 2537 A ₀ .	RL	300	5.0(-4)			2/2	
73 CEH/HEI ¹⁾ At 3130 A ₀ .	RL	300	1.5(-3)			2/2	
73 CEH/HEI ¹⁾ At 3130-3261 A ₀ .	RL	300	4.12(2)			2/1	
The rate ratio to be multiplied by a factor α, dependent on the experimental conditions.							
1) k _{ref} : SO ₂ [*] → products. SO ₂ [*] is a vibrationally excited singlet.							
SO₂^{**} + CO → SO + CO₂							
Sulfur dioxide + Carbon monoxide							
73 CEH/HEI ¹⁾ At 2536 A ₀ .	RL	300	2.24(2)			2/1	1.4
73 CEH/HEI ¹⁾ At 3130 A ₀ .	RL	300	3.37(2)			2/1	1.4
73 CEH/HEI ¹⁾ At 3261 A ₀ .	RL	300	4.68(2)			2/1	1.4
1) k _{ref} : SO ₂ ^{**} → SO ₂ . SO ₂ ^{**} is a chemically active triplet. The rate ratio to be multiplied by a factor β, depending on the experimental conditions.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
SO₂ + CH≡CH → CO + other products						
Sulfur dioxide + Ethyne						
71 FIF/MOR	ES	1500-2150	5.46(11)	0.5	20533	2
The preexponential factor expressed as: A(T/298) ^{0.5} .						
SO₂(³B₁) + CH≡CH → CO + other products						
Sulfur dioxide + Ethyne						
77 SU/CAL	EX	298	1.56(12)			2
Photolysis of SO ₂ /CH≡CH mixtures.						
SO₂(³B₁) + cis-CH₃CH=CHCH₃ → [cis-CH₃CH=CHCH₃.SO₂][*]						
Sulfur dioxide + 2-Butene, (Z)-						
74 DEM/CAL	ES	294	(1.29±0.18)(14)			2
SO₂(³B₁) + trans-CH₃CH=CHCH₃ → [trans-CH₃CH=CHCH₃.SO₂][*]						
Sulfur dioxide + 2-Butene, (E)-						
74 DEM/CAL	ES	294	(1.22±0.15)(14)			2
SO₂(¹B₁) + (CH₃)₃CH → products						
Sulfur dioxide + Propane, 2-methyl-						
78 SU/CAL	EX	298	8.4(12)			2
SO ₂ photolysis. P < 10 torr.						
SO₂(³B₁) + (CH₃)₃CH → products						
Sulfur dioxide + Propane, 2-methyl-						
78 SU/CAL	EX	298	8.7(11)			2
SO ₂ photolysis. P < 10 torr.						
SO₂(³B₁) + cis-CH₃CH₂CH=CHCH₃ → [CH₃CH₂CH=CHCH₃.SO₂][*] → SO₂ + trans-CH₃CH₂CH=CHCH₃						
Sulfur dioxide + 2-Pentene, (Z)-						
76 WAM	ES	295	(6.33±1.25)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{SO}_2(^3\text{B}_1) + \text{trans-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$ $\rightarrow [\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \cdot \text{SO}_2]^*$ $\rightarrow \text{SO}_2 + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$						
Sulfur dioxide + 2-Pentene, (E)- 76 WAM	ES	295	(1.0±0.27)(14)			2
$\text{SO}_3 (+ \text{M}) \rightarrow \text{SO}_2 + \text{O} (+ \text{M})$ Sulfur trioxide 79 AST/GLA M = Ar. Incident or reflected shock-waves. k expressed as k[Ar]. Supersedes 78 AST/GLA. [Ar] = (0.5-4.2) × 10 ¹⁹ molec.cm ⁻³ .						
	EX	1700-2500	3.16(15)	0	31875±1323	2 1.6
$\text{SH} + \text{D}_2 \rightarrow \text{HDS} + \text{D}$ Mercapto + Deuterium molecule 77 FRA/ROG Static system.						
	EX	808-937	1.35(13)	0	3530±220	2 1.8
$\text{SH} + \text{SH} \rightarrow \text{H}_2\text{S} + \text{S}$ Mercapto 72 LAN/OLD Upper-limit k. 73 BRA/TRU 79 NIC/AMO Radio-frequency pulse. Kinetic Spectroscopy. High-vacuum. P = (0.1-2) torr.						
	ES	293	≤1.81(13)			2
	EX	298	7.8(12)			2
	DE	295	(1.9±0.2)(13)			2
$\text{SH} + \text{NO} \rightarrow \text{products}$ Mercapto + Nitrogen oxide (NO) 73 BRA/TRU						
	RN	298	6.3(11)			2
$\text{H}_2\text{S} (+ \text{M}) \rightarrow \text{SH} + \text{H} (+ \text{M})$ Hydrogen sulfide 76 HIG/SAI ¹⁾ 77 BOW/DOD ¹⁾ 82 ROT/LOE1 ¹⁾ Thermolysis behind reflected shock-waves. Atomic Resonance Absorption-Spectroscopy. [H ₂ S] = (0.6-4.9) × 10 ¹⁵ molec.cm ⁻³ . [Ar] = (5.0-8.0) × 10 ¹⁸ molec.cm ⁻³ . P(Total) = (1350-1500) torr.						
	ES	2380-3010	1.26(16)	0	46301	2
	EX	2700-3800	2.00(14)	0	37288±962	2 1.51
	EX	1965-2560	4.64(14)	0	41500	2
1) M = Ar.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$N(^4S) + O_2 \rightarrow NO(v=n) + O$							
Nitrogen atom + Oxygen molecule							
81 RAH/GIB ¹⁾ n = 2.	EX	298	(3.31±0.84)(6)				2
81 RAH/GIB ¹⁾ n = 3.	EX	298	(3.43±0.54)(6)				2
81 RAH/GIB ¹⁾ n = 4.	EX	298	(1.99±0.18)(6)				2
81 RAH/GIB ¹⁾ n = 5.	EX	298	(1.45±0.24)(6)				2
81 RAH/GIB ¹⁾ n = 6.	EX	298	(4.22±1.20)(5)				2
81 RAH/GIB ¹⁾ n = 7.	EX	298	(3.01±1.20)(5)				2
¹⁾ Fourier Transform IR Spectrometry. P(N ₂) = 250 mtorr. P(O ₂) = 500 mtorr.							
$N(^2D) + O_2 \rightarrow NO + O$							
Nitrogen atom + Oxygen molecule							
71 LIN/KAU	EX	300	(3.61±1.20)(12)				2
71 SLA/WOO	EX	237	4.94(12)				2
71 SLA/WOO	EX	295	4.46(12)				2
71 SLA/WOO	EX	365	5.18(12)				2
71 SLA/WOO	EX	1000	8.43(12)				2
Extrapolated rate constant.							
71 SLA/WOO	EX	237-365	4.68(12)	0.5	0		2
The A-factor recalculated from the given T ^{0.5} term and the above experimental rate constants. The preexponential factor expressed as: A(T/298) ^{0.5} .							
72 HUS/KIR2	EX	300	(5.60±1.33)(12)				2
$N(^2P) + O_2 \rightarrow NO + O$							
Nitrogen atom + Oxygen molecule							
72 HUS/KIR2	EX	300	(2.77±1.51)(12)				2
$N + O_2(^1A_g) \rightarrow NO + O$							
Nitrogen atom + Oxygen molecule							
73 SCH/SCH2	EX	300	(1.35±0.52)(9)				2
73 SCH/SCH2	SE	300	1.63(9)				2
Average of present and literature data.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
N + O₃ → NO + O₂ Nitrogen atom + Ozone						
79 STI/PAY Discharge-flow. Flash-photolysis. Resonance-fluorescence. Upper-limit k.	EX	298	<3.01(8)			2
N(²D) + O₃ → NO + O₂ Nitrogen atom + Ozone						
80 HUS/SLA2 UV-photolysis of N ₂ O. Time-resolved Resonance-Fluorescence. Lower-limit k.	EX	300	>2.41(12)			2
N(²D) + H₂ → NH + H Nitrogen atom + Hydrogen molecule						
72 HUS/KIR2	EX	300	(1.02±0.30)(12)			2
N + H₂ (+ M) → NH₂ (+ M) Nitrogen atom + Hydrogen molecule						
81 PET/SAP Discharge-flow. N atoms produced by dissociation of N ₂ in a glow-discharge. Unreported T assumed to be 298 K. Upper-limit k. [H ₂] ~1.3x10 ¹⁷ molec.cm ⁻³ . [M] = 3.6x10 ¹⁷ molec.cm ⁻³ . P(H ₂) = (0.2-0.4) torr.	EX	298	≤3.63(11)			3
N + OH → NO + H Nitrogen atom + Hydroxyl						
77 HAY1 Fuel-rich, Ethylene-, and Acetylene-air flames. k _{ref} : N + NO → N ₂ + O.	RL	1950-2380	(1.0±0.2)			2/2
80 HOW/SMI Discharge-flow. H ₂ O Flash-photolysis. Resonance-fluorescence. P(Total) = 3.75 torr.	EX	298	(3.01±0.72)(13)			2
81 HOW/SMI Discharge-flow. OH radicals formed by H ₂ O Flash- photolysis. N atoms formed by dissociation of ~1% N ₂ in Ar. Resonance-fluorescence. The pre- exponential factor expressed as: A(T/298) ^{-0.25} . [N] = (0.5-5.1)x10 ¹³ molec.cm ⁻³ .	EX	250-515	(3.20±0.27)(13)	-0.25	0	2
81 MOR2 Premixed H ₂ /O ₂ /Ar flames. Laser-fluorescence. P = 760 torr. k _{ref} : N + NO → N ₂ + O.	RL	1790-2200	(1.0±0.3)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
N(²D) + H₂O → products						
Nitrogen atom + Water						
76 SLA/BLA3 Vacuum UV-Photolysis. P(He) = 7 torr. P(N ₂ O + Ar) = 7 torr. (1% N ₂ O in Ar).	EX	198-372	(1.51±0.30)(14)			2
N + SO₃ → NO + SO₂						
Nitrogen atom + Sulfur trioxide						
72 JAC/WIN	EX	300	3.07(8)			2
75 WES/DEH1 Upper-limit k.	EX	298	≤6.0(6)			2
N + N (+ M) → N₂ (+ M)						
Nitrogen atom						
75 BED/TCH M = N ₂ . Electron Paramagnetic Resonance. P = (2.2-3.2) torr.	EX	298	(7.58±1.96)(15)			3
78 EME/MAR ¹ M = Ar.	EX	300	(8.34±1.81)(15)			3
78 EME/MAR ¹ M = He.	EX	300	(7.98±0.73)(15)			3
78 EME/MAR ¹ M = N ₂ .	EX	300	(3.99±1.45)(15)			2
¹) ESR-jet-flow technique. P(Total) = (1.5-8.0) torr.						
79 YAM M = N ₂ . Recombination of N atoms in Lewis-Rayleigh Nitrogen afterglow. P(N ₂) < 4.2 torr.	EX	298	(2.61±0.07)(15)			3
N + NO → N₂ + O						
Nitrogen atom + Nitrogen oxide (NO)						
75 CLY/MCD	EX	298-670	(4.94±0.84)(13)	0	410±120	2
75 CLY/MCD	EX	298	(1.33±0.84)(13)			2
78 LEE/MIC3 Discharge-flow, or Flash-photolysis. Resonance-Fluorescence. T-independent k.	EX	196-400	(2.41±0.12)(13)	0	0	2
79 ISH/SUG1 Pulse-radiolysis. Absorption-spectroscopy. P(Total) = (200-800) torr.	EX	298	(1.39±0.24)(13)			2
80 CHE/CLY Discharge-flow. Resonance-fluorescence.	EX	298	(2.04±0.18)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-1000) torr.	EX	298	(1.14±0.12)(13)			2
N(²D) + NO → N₂ + O						
Nitrogen atom + Nitrogen oxide (NO)						
71 LIN/KAU	EX	300	(4.22±1.51)(13)			2
72 HUS/KIR2	EX	300	(3.67±2.23)(13)			2
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-1000) torr.	EX	298	(2.11±0.18)(13)			2
N(²P) + NO → N₂ + O						
Nitrogen atom + Nitrogen oxide (NO)						
72 HUS/KIR2	EX	300	(2.05±0.66)(13)			2
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-1000) torr.	EX	298	(1.63±0.12)(13)			2
N + NO₂ → N₂O + O (a)						
→ NO + NO (b)						
→ N ₂ + O ₂ (c)						
→ N ₂ + O + O (d)						
Nitrogen atom + Nitrogen oxide (NO ₂)						
75 CLY/MCD k _a .	EX	298	(8.43±0.12)(11)			2
82 CLY/ONO k _a + k _b + k _c + k _d . NO ₂ in excess. Discharge-flow. Resonance-fluorescence. [NO ₂]/[N] ₀ > 80.	EX	293	(1.81±0.19)(12)			2
N(²D) + N₂O → N₂ + NO (a)						
→ N(⁴ S) + N ₂ + O (b)						
Nitrogen atom + Nitrogen oxide (N ₂ O)						
71 SLA/WOO ¹⁾ Preexponential factor expressed as: A(T/298) ^{0.5} .	EX	237-365	3.75(12)	0.5	403±101	2
71 SLA/WOO ¹⁾	EX	300	1.02(12)			2
72 HUS/KIR2 ¹⁾	EX	300	(2.89±0.54)(12)			2
76 SLA/BLA3 ¹⁾ Vacuum-UV Photolysis.	EX	198-372	(6.93±1.81)(12)	0	569±70	2
¹⁾ k _a .						
71 LIN/KAU k _a + k _b .	EX	300	(2.11±0.72)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$N(^2P) + N_2O \rightarrow N_2 + NO$						
Nitrogen atom + Nitrogen oxide (N_2O)						
72 HUS/KIR2	EX	300	(2.05±0.90)(12)			2
$N + HN_3 \rightarrow N_2 + N_2H$						
Nitrogen atom + Hydrazoic acid						
73 LEB/COM	EX	298	2.95(9)			2
$N + NH_2NH_2 \rightarrow NH + NH_2NH$ (a)						
→ products (overall) (b)						
Nitrogen atom + Hydrazine						
75 YO	EX	298	2.7(10)			2
k_a .						
75 YO ¹⁾	EX	298-652	3.1(12)	0	1158	2
75 YO ¹⁾	EX	298	6.7(10)			2
¹⁾ k_b .						
$N + C (+ M) \rightarrow CN(B^2\Sigma^+) (+ M)$						
Nitrogen atom + Carbon atom						
75 WAS/KLE	EX	298	(3.41±0.91)(15)			3
M = Ar. Unreported T assumed to be 298 K.						
74 KLE/WAS	EX	298	3.41(15)			3
M = Ar. Resonance absorption.						
P(Total) = 1torr.						
$N(^2D) + CO_2 \rightarrow NO + CO$ (a)						
→ $N + O + CO$ (b)						
Nitrogen atom + Carbon dioxide						
71 LIN/KAU	EX	300	(3.01±1.20)(11)			2
$k_a + k_b$.						
$N + HCHO \rightarrow$ products						
Nitrogen atom + Formaldehyde						
71 WHI	EX	323-643	2.59(12)	0	1812±302	2
$N + CH_3OH \rightarrow HNO + CH_3$						
Nitrogen atom + Methanol						
73 ROS/ROS	EX	309-409	2.40(11)	0	4330±481	2 1.20
P = (1.07-1.56) torr.						
73 ROS/ROS	RL	299-306	(3.6±0.4)	0	0	2/2
k_{ref} : $N + CH_3OD \rightarrow$ products.						
73 ROS/ROS	RL	340-346	(8.0±1.0)	0	0	2/2
k_{ref} : $N + CD_3OD \rightarrow$ products.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
N + CH₃OD → DNO + CH₃							
Nitrogen atom + Methanol-d							
73 ROS/ROS ¹⁾ Average of 4 k's. P = (1.08-1.92) torr.	EX	299-306	(5.3±1.2)(7)	0	0	2	
73 ROS/ROS ¹⁾ Average of 3 k's. P = (1.08-1.12) torr.	EX	340-346	(1.25±0.15)(8)	0	0	2	
¹⁾ [CH ₃ OD] = (1.50-4.54) × 10 ¹⁸ molec. cm ⁻³ .							
N + CN → C + N₂							
Nitrogen atom + Cyanogen							
76 SLA	ES	5000-8000	(4.4±2.0)(14)	0	4529	2	
N + CH=CH → products							
Nitrogen atom + Ethyne							
77 MIC/LEE Discharge-flow. Resonance-fluorescence. Upper-limit k. P = (1.5-2.5) torr.	EX	298	<3.01(8)			2	
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(1.02±0.12)(10)			2	
N + CH₂=CH₂ (+ M) → products							
Nitrogen atom + Ethene							
77 MIC/LEE Discharge-flow. Resonance-fluorescence. Upper-limit k. P = (1.5-2.5) torr. [N] ₀ ~ 1.0 × 10 ¹² molec. cm ⁻³ .	EX	298	<3.01(8)			2	
79 ISH/SUG1 Pulse-radiolysis. Absorption-spectroscopy. Upper-limit k. P(Total) = (200-800) torr.	EX	298	≤3.98(10)			2	
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(3.91±0.78)(10)			2	
80 HUS/SLA2 M = N ₂ . N ₂ O photolysis. Resonance-fluorescence.	EX	300	(3.41±0.22)(17)			3	
N(²D) + CH₂=CH₂ → products							
Nitrogen atom + Ethene							
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-800) torr.	EX	298	(2.23±0.18)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
N(²P) + CH₂=CH₂ → products						
Nitrogen atom + Ethene						
80 SUG/ISH2 Pulse-radiolysis. Resonance-absorption. P(Total) = (200-700) torr.	EX	298	(1.69±0.12)(13)			2
N + CH₃CH₂OH → HNO + CH₃CH₂						
Nitrogen atom + Ethanol						
73 ROS/ROS [CH ₃ CH ₂ OH] = (1.45-4.76)x10 ¹⁸ molec.cm ⁻³ . P = (1.12-1.63) torr.	EX	312-425	2.00(11)	0	4210±241	2 1.10
N + CH₃C≡CH → products						
Nitrogen atom + 1-Propyne						
77 MIC/LEE Discharge-flow. Resonance-fluorescence. Upper-limit k. P = (1.5-2.5) torr. [N] ₀ ~ 1.0x10 ¹² molec.cm ⁻³ .	EX	298	<3.01(8)			2
N + CH₃CH=CH₂ → products						
Nitrogen atom + 1-Propene						
77 MIC/LEE Discharge-flow. Resonance-fluorescence. Upper-limit k. P = (1.5-2.5) torr. [N] ₀ ~ 1.0x10 ¹² molec.cm ⁻³ .	EX	298	<3.01(8)			2
79 SAT/SUG Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.	EX	300	(6.63±1.20)(10)			2
N + CH₃CH₂CH₂OH → HNO + CH₃CH₂CH₂						
Nitrogen atom + 1-Propanol						
73 ROS/ROS [CH ₃ CH ₂ OH] = (0.93-3.80)x10 ¹⁸ molec.cm ⁻³ . P = (1.29-1.48) torr.	EX	354-494	2.75(11)	0	3609±241	2 1.10
N + (CH₃)₂CHOH → HNO + (CH₃)₂CH						
Nitrogen atom + 2-Propanol						
73 ROS/ROS [CH ₃ CH ₂ OH] = (0.38-1.22)x10 ¹⁸ molec.cm ⁻³ . P = (0.865-1.73) torr.	EX	304-449	8.51(11)	0	4691±241	2 1.12

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err.
N + CH₂-CH=CH-CH₂ → products							
Nitrogen atom + 1,3-Butadiene							
79 SAT/SUG	EX	300	(6.63±0.60)(10)			2	
Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.							
N + CH₃CH₂CH=CH₂ → products							
Nitrogen atom + 1-Butene							
79 SAT/SUG	EX	300	(6.63±0.60)(10)			2	
Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.							
N + cis-CH₃CH=CHCH₃ → products							
Nitrogen atom + 2-Butene, (Z)-							
79 SAT/SUG	EX	300	(3.91±0.48)(10)			2	
Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.							
N + trans-CH₃CH=CHCH₃ → products							
Nitrogen atom + 2-Butene, (E)-							
79 SAT/SUG	EX	300	(4.04±0.54)(10)			2	
Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.							
N + (CH₃)₂C=CH₂ → products							
Nitrogen atom + 1-Propene, 2-methyl-							
79 ISH/SUG1	EX	298	≤8.43(10)			2	
Pulse-radiolysis. Absorption-spectroscopy. Upper-limit k. P(Total) = (200-600) torr.							
79 SAT/SUG	EX	300	(1.08±0.12)(11)			2	
Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.							
N + NCC=CCN → [N.C₄N₂†]							
Nitrogen atom + 2-Butynedinitrile (Dicyanoacetylene)							
72 HAN/OBE2	ES	300	(3.19±2.59)(9)			2	
N + (CH₃)₂C=CHCH₃ → products							
Nitrogen atom + 2-Butene, 2-methyl-							
79 SAT/SUG	EX	300	(4.94±0.48)(10)			2	
Pulse-radiolysis. Resonance-absorption. P(N ₂) = (200-600) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$N_2 (+M) \rightarrow N + N (+M)$							
Nitrogen molecule							
74 KEW/HOR ¹⁾ M = N.	EX	6000-14000	5.54(19)	-2.5	113200	2	1.58
74 KEW/HOR ¹⁾ M = N ₂ .	EX	6000-14000	5.03(20)	-3.5	113200	2	1.58
¹⁾ The preexponential factor expressed as: A(T/298) ⁿ .							
$N_2(A^3\Sigma_u^+) + O_2 \rightarrow N_2(X^1\Sigma) + O_2^*$ (a)							
$\rightarrow N_2(X^1\Sigma) + O(^1P) + O(^1P)$ (b)							
$\rightarrow N_2O(X^2\Pi) + O(^3P)$ (c)							
$\rightarrow N_2O(X^2\Pi) + O(^1D)$ (d)							
Nitrogen molecule + Oxygen molecule							
82 IAN/JEF ¹⁾ k _a .	ES	298	≈6.02(11)			2	
82 IAN/JEF ¹⁾ k _b .	ES	298	≈1.20(12)			2	
82 IAN/JEF ¹⁾ k _c + k _d .	ES	298	≈3.61(10)			2	
82 IAN/JEF ¹⁾ k _a + k _b + k _c + k _d .	EX	298	1.81(12)			2	
¹⁾ M = Ar. Discharge-flow. Laser-induced fluorescence. Weighted average k's. P(Total) ~ 2 torr.							
$N_2(A^3\Sigma_u^+, v=n) + O_2 \rightarrow \text{products}$							
Nitrogen molecule + Oxygen molecule							
81 IAN/KAU ¹⁾ n = 0.	EX	298	(1.51±0.24)(12)			2	
81 IAN/KAU ¹⁾ n = 1.	EX	298	(2.35±0.36)(12)			2	
81 IAN/KAU ¹⁾ n = 2.	EX	298	(2.59±0.42)(12)			2	
¹⁾ Discharge-flow. Laser-induced fluorescence.							
$N_3 + N_3 \rightarrow N_2 + N_2 + N_2$							
Azide							
79 JOU/LEB1 Calculation based on computer simulation.	DE	298	(3.91±0.90)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NO (+ M) → N + O (+ M)						
Nitrogen oxide (NO)						
73 MYE M = Ar.	EX	2600-6300	1.37(14)	0	74685	2
73 MYE M = NO. Upper-limit estimate.	ES	2600-6300	≤3.0(14)	0	76497	2
NO + O₂(¹Δ_g) → NO₂ + O						
Nitrogen oxide (NO) + Oxygen molecule						
76 DUM	EX	298	2.94(6)			2
NO + NO → N₂ + O₂ (a)						
→ N₂O + O (b)						
Nitrogen oxide (NO)						
75 TRU/MAC k _a . M = Ne. The preexponential factor expressed as: A(T/298) ^{0.5} .	EX	2700-4700	3.07(12)	0.5	30458	2
73 MYE k _b .	EX	2595-6300	2.35(10)	0	14595	2
76 MCC/KRU k _b . Best fit to the experimental data.	EX	1750-2100	1.80(12)	0	32109	2 2.04
77 MCC/KRU k _b . Flow reactor.	EX	1750-2100	1.80(12)	0	32109	2 2.0
79 KOS/ASA k _b . Incident shock-waves. Computer simulation. [NO] = (2.4-4.2) × 10 ¹⁸ molec. cm ⁻³ . P ₀ = 30 torr.	DE	2700-3500	4.9(12)	0	33770	2
NO + NO + NO → NO₂ + N₂O						
Nitrogen oxide (NO)						
79 GVO/NES1 ¹⁾ P = (6.0- 10.5) torr.	EX	753-813	1.26(10)	0	13589±1007	3 2.88
79 GVO/NES2 ¹⁾ P = (22.5-112.5) torr.	EX	713-923	1.07(10)	0	13488±151	3 1.15
¹⁾ NO oxidation in a stainless-steel vessel.						
NO + NO + O₂ → NO₂ + NO₂						
Nitrogen oxide (NO) + Oxygen molecule						
73 STE/NIK1	EX	298	(1.45±0.07)(10)			3
75 ENG/COR	EX	298	(1.46±0.03)(10)			3
75 ENG/COR	EX	298-323	(1.99±0.28)(9)	0	-591±43	3
A and B recalculated from the reported data.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
NO + NO₂ + H₂O → HONO + HONO							
Nitrogen oxide (NO) + Nitrogen oxide (NO ₂) + Water							
75 ENG/COR Best data-fit by optimization.	ES	298-323	(1.5±0.5)(11)	0	0	3	
76 CHA/NOR k ₁ = Kk ₋₁ .	DE	296	(2.19±0.70)(10)			3	
NO + NO₃ → NO₂ + NO₂							
Nitrogen oxide (NO) + Nitrogen oxide (NO ₂)							
73 HAR/JOH	RN	296	5.24(12)			2	
74 GLA/TRO1 Best fit to the experimental data.	ES	1000-1100	(8.0±4.0)(12)			2	
75 GRA k ₁ = Kk ₋₁ .	DE	297	(1.13±0.25)(13)			2	
78 GRA/JOH Modulated photolysis technique. k ₁ = k ₋₁ K.	DE	297	(1.14±0.24)(13)			2	
NO + N₂O → NO₂ + N₂							
Nitrogen oxide (NO) + Nitrogen oxide (N ₂ O)							
73 BOR/SKA	ES	1050-2510	2.75(14)	0	25164±1510	2	1.58
79 GVO/NES3 N ₂ O decomposition in a stainless-steel vessel under static conditions. Gas-chromatography. P = (22.5-112.5) torr.	EX	713-923	1.51(11)	0	24811±302	2	2.51
NO + NH₂ → N₂ + H₂O							
Nitrogen oxide (NO) + Amidogen							
71 GOR/MUL Unreported T assumed to be 298 K.	EX	298	1.6(13)			2	
72 BED/THO k _{ref} : NH ₂ + NO ₂ → NH + HONO.	RL	615-660	5.01(-3)	0	-3221±503	2/2	
73 GEH/HOY The water molecule formed as product is vibrationally excited.	EX	298	(5.0±1.0)(12)			2	
NO + NH₃ → HNO + NH₂							
Nitrogen oxide (NO) + Ammonia							
78 ROO/HAN Shock-waves.	ES	1700-3000	5.0(14)	0	25164	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A k err. units factor
NO + HNO → products						
Nitrogen oxide (NO) + Nitrosyl hydride						
81 CHE/NAD CH ₃ CHO/NO flash-photolysis. P(HCHO) = 7 torr. P(CH ₃ CHO) = 12.2 torr. P(NO) = (20-380) torr.	EX	298	(3.01±0.90)(5)			2
NO + HONO₂ → NO₂ + HONO						
Nitrogen oxide (NO) + Nitric acid						
77 KAI/WU	EX	300	9.03(3)			2
79 MCK/MAT Flow-reactor. Spectrophotometry. P = 760 torr.	EX	298	8.4(3)			2
79 STR/WEL Tunable diode-laser. Static reactor.	EX	296	(2.05±1.20)(2)			2
NO + C₂O → NCO + CO (a) → CNO + CO (b)						
Nitrogen oxide (NO) + Carbon oxide (C ₂ O)						
80 DON/PIT k _a + k _b . Laser photodissociation of C ₃ O ₂ nm. Dye-laser induced fluorescence.	EX	298	(2.61±0.07)(13)			2
NO₂ (+ M) → NO + O (+ M)						
Nitrogen oxide (NO ₂)						
79 END/GLA M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.61(Ar), 0.61(Kr), 0.69(Xe), 0.82(Ne), 2.04(CO ₂), 2.04(CF ₄), 2.14(He). Thermolysis in shock-waves. Rate constants expressed as k[M].	EX	1800	2.45(8)			2
NO₂ + NO₂ → NO + NO₃ (a) → NO + anti-NO₃ (b)						
Nitrogen oxide (NO ₂)						
73 BUT/LEV k _a .	ES	1700-2400	(3.2±1.0)(12)	0	12870	2
77 FRE/PAL k _b .	ES	1471-1855	3.16(13)	0	17111	2
NO₂ + NO₂ + CH₃OH → HONO₂ + CH₃ONO						
Nitrogen oxide (NO ₂) + Methanol						
82 NIK/MAK1 FTIR-spectroscopy. P(CH ₃ OH) = (0-1.0) torr. P(NO ₂) = (0-1.0) torr. P(N ₂) = 700 torr.	EX	298	(2.07±0.22)(11)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{NO}_2 + \text{NO}_2 + \triangle \rightarrow \text{products}$						
Nitrogen oxide (NO_2) + Oxirane						
71 JAF Preliminary results.	EX	298-373	1.3(12)	0	1862	3
$\text{NO}_2 + \text{NO}_2 + \text{CH}_3\text{CH}_2\text{OH} \rightarrow \text{HONO}_2 + \text{CH}_3\text{CH}_2\text{ONO}$						
Nitrogen oxide (NO_2) + Ethanol						
82 NIK/MAK1 FTIR-spectrometry. $P(\text{CH}_3\text{CH}_2\text{OH}) = (0.1-1.0)$ torr. $P(\text{NO}_2) = (0-1.0)$ torr. $P(\text{N}_2) = 700$ torr.	EX	298	(2.07±0.29)(11)			3
$\text{NO}_2 + \text{NO}_3 (+M) \rightarrow \text{NO} + \text{NO}_2 + \text{O}_2 (+M)$ (a) $\rightarrow \text{N}_2\text{O}_5 (+M)$ (b)						
Nitrogen oxide (NO_2) + Nitrogen oxide (NO_3)						
75 GRA k_a . $k_a = k_{-a}K$.	DE	298-329	(1.51±0.30)(10)	0	1228±101	2
78 GRA/JOH k_a . Modulated photolysis. $k_a = k_{-a}K$.	DE	298-329	(1.51±0.30)(10)	0	1230±100	2
80 CON k_b . $M = \text{N}_2$. Limiting high-pressure k . $\text{N}_2\text{O}_5/\text{NO}$ thermolysis. $[\text{N}_2] < 2 \times 10^{18}$ molec. cm^{-3} .	EX	262-272	1.28(14)	0	1360	2
82 FOW/MIT k_b . Closed system. NO_3 generated by injecting NO_2 in a O_3 flow. k expressed as $k[M]$. $[\text{NO}_2]_0 = (0.1-1.0) \times 10^{13}$ molec. cm^{-3} . $[\text{O}_3] = (5.5-7.4) \times 10^{17}$ molec. cm^{-3} .	EX	298	(1.20±0.48)(12)			2
82 MAL/TRO k_b . Limiting high-pressure k . Recommended k , in terms of unimolecular rate theory. The pre- exponential factor expressed as: $A(T/298)^{0.2}$.	RE	200-300	9.62(11)	0.2	0	2
80 CON k_b . $M = \text{N}_2$. Limiting low-pressure k . $\text{N}_2\text{O}_5/\text{NO}$ Thermolysis. 10^{18} molec. cm^{-3} .	EX	268-307	3.48(15)	0	-1550	3
78 WAY/MIT k_b . Flow-reactor. $M = \text{NO}_2, \text{O}_2$. Preliminary k .	ES	298	1.31(16)			3
82 MAL/TRO k_b . Rate constant expressed as $k/[M]$. Limiting low-pressure k . Recommended k , evaluated in terms of unimolecular rate theory. The pre- exponential factor expressed as $A(T/298)^{-4.1}$.	RE	200-300	1.38(18)	-4.1	0	3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
NO₂ + NH₃ → HONO + NH₂						
Nitrogen oxide (NO ₂) + Ammonia						
72 BED/THO Cylindrical Pyrex reaction vessel. Photomultiplier. Logarithmic amplifier.	EX	615-660	3.98(12)	0	13916±51	2 2.0
NO₂ + HONO → NO + HONO₂						
Nitrogen oxide (NO ₂) + Nitrous acid						
79 STR/WEL Tunable diode-laser. Static reactor. k ₁ = k ₋₁ K.	DE	296	≤6.02(1)			2
NO₂ + CH₄ → HONO + CH₃						
Nitrogen oxide (NO ₂) + Methane						
78 SLA/GRI3 Shock-waves. P = (2-4) Atm.	ES	1300-1900	7.0(11)	0	15098	2
81 SLA/GRI CH ₄ /O ₂ /Ar ignition sensitized by NO ₂ behind reflected shock-waves. P = (1.8-3.6) atm.	ES	1310-1790	1.2(13)	0	15098	2
NO₂ + HCN → HONO + CN (a) → HNO + NCO (b)						
Nitrogen oxide (NO ₂) + Hydrocyanic acid						
82 FIF/HOL ¹⁾	EX	1300	≤1.0(7)			2
82 FIF/HOL ¹⁾	EX	1800	≤1.0(10)			2
¹⁾ k _a = k _b . Reaction behind shock-waves in Ar. Upper-limit k's. P = (1.7-12.6) atm.						
NO₂ + CH₂=CH₂ → products						
Nitrogen oxide (NO ₂) + Ethene						
71 JAF	EX	298-373	2.00(6)	0	4145	2
71 JAF	EX	298	1.82			2
NO₂ + CH₃CHO → HONO + CH₃CO						
Nitrogen oxide (NO ₂) + Acetaldehyde						
71 JAF	EX	298-373	1.58(5)	0	3473	2
71 JAF	EX	298	1.50			2
72 DAV/COR	EX	295	(8.596±0.189)			2
72 DAV/COR The A-factor recalculated from the reported experimental data.	EX	295-395	3.10(10)	0	6492±302	2
74 JAF/WAN	EX	295-390	2.51(10)	0	6241	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
NO₂ + CH₃C≡CH → products							
Nitrogen oxide (NO ₂) + 1-Propyne							
73 ASH/THO	EX	443-493	4.68(8)	0	6427±81	2	1.20
NO₂ + CH₃CH=CH₂ → products							
Nitrogen oxide (NO ₂) + 1-Propene							
71 JAF	EX	298-373	3.2(6)	0	3914	2	
71 JAF	EX	298	6.24			2	
76 GRY/ROZ	EX	293-373	2.4(5)	0	2818	2	
NO₂ + CH₃CH₂CH₃ → HONO + (CH₃)₂CH							
Nitrogen oxide (NO ₂) + Propane							
76 TIT/BAL	EX	423-498	2.40(11)	0	11374±60	2	1.12
NO₂ + CH₃CH₂CHO → HONO + CH₃CH₂CO							
Nitrogen oxide (NO ₂) + Propanal							
74 JAF/WAN	EX	295-390	2.51(10)	0	6241	2	
NO₂ + (CH₃)₂CO → HONO + CH₃COCH₂							
Nitrogen oxide (NO ₂) + 2-Propanone							
71 JAF	EX	298-373	3.8(5)	0	3588	2	
71 JAF	EX	298	2.4			2	
NO₂ + CH₂=CHC≡CH → products							
Nitrogen oxide (NO ₂) + 1-Buten-3-yne							
75 GRY/ROZ	EX	273-333	8.8(5)	0	1711	2	
NO₂ + CH₃C≡CCH₃ → products							
Nitrogen oxide (NO ₂) + 2-Butyne							
73 ASH/THO	EX	443-493	3.63(8)	0	6029±96	2	1.23
NO₂ + CH₃CH₂CH=CH₂ → products							
Nitrogen oxide (NO ₂) + 1-Butene							
71 JAF	EX	298-373	2.51(6)	0	3684	2	
71 JAF	EX	298	1.07(1)			2	
NO₂ + cis-CH₃CH=CHCH₃ → products							
Nitrogen oxide (NO ₂) + 2-Butene, (Z)-							
71 JAF	EX	298-373	2.51(5)	0	2763	2	
71 JAF	EX	298	2.36(1)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NO₂ + trans-CH₃CH=CHCH₃ → products						
Nitrogen oxide (NO ₂) + 2-Butene, (E)-						
71 JAF	EX	298-373	1.58(6)	0	3224	2
71 JAF	EX	298	3.17(1)			2
NO₂ + (CH₃)₂C=CH₂ → products						
Nitrogen oxide (NO ₂) + 1-Propene, 2-methyl-						
71 JAF	EX	298-373	3.98(4)	0	1980	2
71 JAF	EX	298	5.17(1)			2
NO₂ + CH₃CH₂CH₂CHO → HONO + CH₃CH₂CH₂CO						
Nitrogen oxide (NO ₂) + Butanal						
74 JAF/WAN	EX	295-390	2.51(10)	0	6241	2
NO₂ + CH₃CH₂N(10)=CHCH₃ → NO + CH₃CH₂NO + CH₃CHO						
Nitrogen oxide (NO ₂) + Ethanamine, N-ethylidene- N-oxide						
82 GLE/HEI ¹⁾ Lower-limit k.	EX	298	>6.02(7)			2
82 GLE/HEI ¹⁾ k _{ref} : (CH ₃ CH ₂) ₂ NO + CH ₃ CH ₂ N(10)=CHCH ₃ → adduct	RL	298	3.0(-1)			2/2
¹⁾ Diethylhydroxylamine oxidation by NO ₂ in a IR gas-cell. [NO ₂] (15-236) mtorr. [HONO] = (11-15) mtorr. [(CH ₃ CH ₂) ₂ NOH] = (25-45) mtorr.						
NO₂ + (CH₃CH₂)₂NOH → HONO + (CH₃CH₂)₂NO (a) → any other products (b)						
Nitrogen oxide (NO ₂) + Ethanamine, N-ethyl-N-hydroxy-						
82 GLE/HEI k _a . Diethylhydroxylamine oxidation by NO ₂ in a IR gas-cell. [NO ₂] (15-236) mtorr. [HONO] = (11-15) mtorr. [(CH ₃ CH ₂) ₂ NOH] = (25-45) mtorr.	ES	298	(3.31±0.60)(6)			2
74 JAY/SIM k _{overall} . Dark reaction of (CH ₃ CH ₂) ₂ NOH (diluted in CO ₂) with NO ₂ (diluted in O ₂). High-vacuum. P(Diethylhydroxylamine) = 2.2 mtorr. P(NO ₂) = 19.3 mtorr.	EX	298	2.71(6)			2
NO₂ + CH₂=CHC(CH₃)=CH₂ → products						
Nitrogen oxide (NO ₂) + 1,3-Butadiene, 2-methyl-						
75 GRY/ROZ	EX	273-433	1.7(7)	0	1056	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NO₂ + CH₃CH₂CH₂CH=CH₂ → products						
Nitrogen oxide (NO ₂) + 1-Pentene						
71 JAF	EX	298-373	1.58(6)	0	3684	2
71 JAF	EX	298	6.76			2
NO₃ + NO₃ → NO₂ + NO₂ + O₂						
Nitrogen oxide (NO ₃)						
75 GRA	EX	298-329	(5.12±1.69)(11)	0	2451±101	2
78 GRA/JOH	EX	298-329	(5.12±1.69)(11)	0	2450±100	2
Modulated photolysis.						
80 AFA/DOR	CO	300-350	(1.69±0.24)(12)	0	3400±600	2
Given with caution.						
Indirect measurement based on the literature data for the reaction:						
$\text{NO}_2 + \text{O}_3 \rightarrow \text{NO}_3 + \text{O}_2$						
and K for reaction:						
$\text{N}_2\text{O}_5 = \text{NO}_2 + \text{NO}_3$.						
NO₃ + CH₂=CH₂ → products						
Nitrogen oxide (NO ₃) + Ethene						
75 JAP/NIK	EX	300	(5.60±0.60)(8)			2
Data fit to a proposed mechanism.						
NO₃ + CH₃CHO → HONO₂ + CH₃CO						
Nitrogen oxide (NO ₃) + Acetaldehyde						
74 MOR/NIK	EX	300	7.23(8)			2 1.25
Best fit of experimental data.						
NO₃ + CH₃CH=CH₂ → products						
Nitrogen oxide (NO ₃) + 1-Propene						
75 JAP/NIK	EX	300	(3.19±0.18)(9)			2
Data fit to a proposed mechanism.						
NO₃ + CD₃CD=CD₂ → products						
Nitrogen oxide (NO ₃) + 1-Propene-d ₆						
75 JAP/NIK	EX	300	(3.55±0.24)(9)			2
Data fit to a proposed mechanism.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A k err. units factor
NO₃ + CH₃CH₂CH=CH₂ → products						
Nitrogen oxide (NO ₃) + 1-Butene						
75 JAP/NIK Data fit to a proposed mechanism.	EX	300	(4.69±0.48)(9)			2
NO₃ + cis-CH₃CH=CHCH₃ → products						
Nitrogen oxide (NO ₃) + 2-Butene, (Z)-						
75 JAP/NIK Data fit to a proposed mechanism.	EX	300	(1.08±0.12)(11)			2
NO₃ + trans-CH₃CH=CHCH₃ → products						
Nitrogen oxide (NO ₃) + 2-Butene, (E)-						
75 JAP/NIK Data fit to a proposed mechanism.	EX	300	(8.43±0.60)(10)			2
NO₃ + (CH₃)₂C=CH₂ → products						
Nitrogen oxide (NO ₃) + 1-Propene, 2-methyl-						
75 JAP/NIK Data fit to a proposed mechanism.	EX	300	(6.63±0.60)(10)			2
NO₃ + CH₃CH=C(CH₃)₂ → products						
Nitrogen oxide (NO ₃) + 2-Butene, 2-methyl-						
75 JAP/NIK Data fit to a proposed mechanism.	EX	300	(3.31±0.30)(12)			2
NO₃ + (CH₃)₂C=C(CH₃)₂ → products						
Nitrogen oxide (NO ₃) + 2-Butene, 2,3-dimethyl-						
75 JAP/NIK Data fit to a proposed mechanism.	EX	300	(2.23±0.30)(13)			2
N₂O (+ M) → N₂ + O (+ M) (a)						
→ any other products (b)						
Nitrogen oxide (N ₂ O)						
71 D'A k _a . M = Ar. Rate constant expressed as: k/[M].	EX	1600-2500	2.88(1)	0	27680	2
71 LIP k _a . M = Kr.	EX	1400-2000	1.35(13)	0	24555±2235	2 3.98
72 BOR/SKA k _a . M = Ar + N ₂ . Reflected shock-waves.	EX	1000-2000	5.01(14)	0	28686±755	2 2.0
72 SOL k _a . M = N ₂ O.	SE	1000-3000	4.7(14)	0	29190	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 VER/KIS k _a . M = N ₂ . Limiting high-pressure k.	EX	1250-1800	1.4(11)	0	26573	1	
73 LIP/MIL k _a . M = Kr.	EX	1300-1950	1.26(13)	0	22194	2	
75 BAB/DEA k _a . M = Ar.	EX	1850-2535	7.83(14)	0	28628	2	
75 DOV/NIP k _a . M = Ar.	EX	2160-2500	5.01(13)	0	29190	2	
76 DEA k _a . Data fit to a proposed mechanism.	ES	1950-3075	1.96(14)	0	25861	2	
77 BAL/VAN k _a . M = H ₂ . Supersonic molecular beam. Mass-spectrometry. P = 40 torr.	EX	1670-1980	(1.3±0.4)(15)	0	28435	2	
77 DEA/STE1 k _a . M = Ar. Shock-waves. N ₂ O/CO/Ar mixtures at a total concentration of (2.5-7.7)×10 ¹⁸ molec.cm ⁻³ .	EX	2100-3200	2.71(14)	0	27184	2	
77 MON/HAN1 k _a . M = Ar, Kr, N ₂ , or O ₂ . Best data-fit.	ES	1815-3365	1.42(14)	0	25808	2	1.5
79 END/GLA k _a . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.52(Xe), 0.61(Kr), 0.78(Ar), 1.48(Ne), 4.26(He), 4.81(CF ₄). Thermolysis in shock-waves. Rate constants expressed as k[M].	EX	2000	2.7(8)			2	
80 SUL/KLI k _a . M = Ar. Thermolysis behind shock-waves. P = (1300-3500) torr.	EX	1685-2560	(3.71±2.74)(14)	0	13920±727	2	
80 ZAS/LOS k _a . M = Ar. M-efficiencies relative to Ar are: 1.00(Ar), 2.0(N ₂), 3.0(CO), 4.0(He). [Ar] = (0.6-1.4)×10 ¹⁹ molec.cm ⁻³ . Thermolysis of N ₂ in Ar, He, N ₂ , or CO, behind shock-waves.	EX	1700-2500	4.4(14)	0	28183	2	
71 LIP k _{overall} . M = Kr.	EX	1400-2000	3.09(12)	0	20493±1550	2	3.98
73 VOM2 k _{overall} . M = Ne. Low-pressure k.	EX	1800-2400	3.16(13)	0	21641±2013	2	2.51
74 TRA 1) k _{overall} . Shock-tube. Unspecified high-T range.	EX	1)	3.63(14)	0	26724	2	
75 BAB/DEA k _{overall} .	EX	1850-2525	2.95(14)	0	26355±625	2	1.32
76 DEA 2) Without added H ₂ .	EX	1950-3075	1.15(14)	0	24478±433	2	1.20

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 DEA ²⁾ With 0.01% H ₂ added. ²⁾ k _{overall} .	EX	1950-3075	5.25(13)	0	22072±433	2	1.20
N₂O₅ (+ M) → NO₂ + NO₃ (+ M) (a) → any other products (b)							
Nitrogen oxide (N ₂ O ₅)							
79 CON/JOH ¹⁾ k _a . M = N ₂ . Limiting high-pressure k.	EX	262-345	1.78(17)	0	12540±130	1	
80 CON ²⁾ k _a . M = N ₂ . Limiting high-pressure k.	EX	268-307	1.78(17)	0	12540±200	1	
81 VIG/DAV ²⁾ k _a . Troe fit. Limiting high-pressure k.	RE	285-384	1.21(17)	0	12662±322	1	
81 VIG/DAV ³⁾ k _a . Johnston fit. Limiting high-pressure k.	EX	285-384	1.8(17)	0	12788±242	1	
82 FOW/MIT k _a . M = O ₂ . NO ₃ generated by injecting NO ₂ in a O ₃ flow. k expressed as k[M]. [O ₂] = (2.7-5.1) × 10 ¹⁸ molec. cm ⁻³ . [NO ₂] ₀ > 1.0 × 10 ¹⁴ molec. cm ⁻³ .	EX	298	(1.0±0.6)(-1)			1	
82 MAL/TRO ⁴⁾ k _a . M = N ₂ . Limiting high-pressure k.	TH	220-300	9.69(14)	0.1	11080	1	
79 CON/JOH ¹⁾ k _a . M = N ₂ . Limiting low-pressure k. ¹⁾ quartz reactor. IR-Spectrometry.	EX	262-345	3.67(18)	0	9570±200	2	
80 CON ²⁾ k _a . M = N ₂ . Limiting low-pressure k. ²⁾ N ₂ O ₅ Thermolysis in presence of NO. [N ₂] < 2 × 10 ¹⁸ molec. cm ⁻³ .	EX	268-307	4.85(18)	0	9630±200	2	
81 VIG/DAV ³⁾ k _a . Troe fit. Limiting low-pressure k.	RE	285-384	6.93(18)	0	9914±453	2	
81 VIG/DAV ³⁾ k _a . Johnston fit. Limiting low-pressure k. ³⁾ Flowing-afterglow. Mass-spectrometry. Data-fit to theoretical models. P = (10-800) torr.	EX	285-384	3.28(18)	0	9653±292	2	
82 MAL/TRO ⁴⁾ k _a . M = N ₂ . Rate constant expressed as k/[M]. Limiting-low-pressure k. ⁴⁾ Critical evaluations. The preexponential factor expressed as: A(T/298) ⁿ .	TH	220-300	1.36(21)	-4.4	11080	2	
72 DUT/BUN k _{overall} . Preliminary rate constant.	EX	308	(1.11±0.21)(-4)			1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
NH + O ₂ → NO + OH (a)							
→ NO ₂ + H (b)							
→ HNO + O (c)							
Imidogen + Oxygen molecule							
79 PAG/ERI	ES	300	≤2.0(10)			2	
k _a . Gaseous NH ₃ pulse-radiolysis. Upper-limit k.							
78 ZET/HAN	EX	296	(5.12±0.54)(9)			2	
k _a + k _b + k _c . Resonance-fluorescence. UV-photo- lysis. Channel (c) is the most probable path.							
NH + H ₂ → NH ₂ + H							
Imidogen + Hydrogen molecule							
79 DOV/NIP ¹⁾	EX	2601	1.8(12)			2	
79 DOV/NIP ¹⁾	EX	2788	2.2(12)			2	
¹⁾ Pyrolysis behind reflected shock-waves.							
NH + N ₂ (+ M) → HN ₃ (+ M) (a)							
→ any other products (b)							
Imidogen + Nitrogen molecule							
81 ZET/STU	EX	298	<3.63(9)			3	
k _a . M = N ₂ . Pulsed vacuum-UV photolysis of NH ₃ at 105 nm. Resonance-fluorescence. Upper-limit k. P(NH ₃) = (0.005-0.9) torr. P(N ₂) < 900 torr.							
81 ZET/STU	EX	298	<1.81(5)			2	
k _{overall} . Pulsed vacuum-UV photolysis of NH ₂ at 105 nm. Resonance-fluorescence. Upper-limit k. P(NH ₃) = (0.005-0.9) torr.							
NH + NO → H + N ₂ O (a)							
→ any other products (b)							
Imidogen + Nitrogen oxide (NO)							
78 ROO/HAN ¹⁾	ES	1700-3000	6.46(11)	0.75	0	2	
k _a . Shock-waves. The preexponential factor expressed as: A(T/298) ^{0.75} .							
81 ROO/HAN ¹⁾	EX	1760-2850	8.0(13)	0	14800	2	3.0
k _a . Best data-fit.							
¹⁾ NH ₃ /NO, or N ₂ O in Ar behind incident shock-waves. Emission and IR-laser Absorption.							
71 GOR/MUL	EX	298	2.3(13)			2	
k _{overall} . Unreported T assumed to be 298 K.							
76 HAN/HOE	EX	298	(2.83±0.72)(13)			2	
k _{overall} . Unreported T assumed to be 298 K.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 MOR2 k _{overall} . Premixed H ₂ /O ₂ /Ar Flames. Laser-Fluorescence. Upper-limit k. P = 760 torr.	EX	1790	<4.22(12)			2	
NH + NH₂ → NH₂NH							
Imidogen + Amidogen							
79 PAG/ERI Gaseous NH ₃ pulse-radiolysis.	EX	349	7.0(13)			2	
NH + NH₃ (+ M) → NH₂NH₂ (+ M) (a) → any other products (b)							
Imidogen + Ammonia							
81 ZET/STU ¹⁾ k _a . M = N ₂ . M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.06(He) 1.00(Ar), 60.22(NH ₃). P(M) <900 torr.	EX	298	<1.8(13)			3	
81 ZET/STU ¹⁾ k _{overall} . ¹⁾ Pulsed vacuum-UV Photolysis of NH ₃ at 105 nm. Resonance-fluorescence. P(NH ₃) = (0.05-0.9) torr.	EX	298	<4.82(7)			2	
NH(a¹Δ) + HN₃(¹A') → NH₂(²A₁) + N₃(²Π_g) (a) → NH(X ³ Σ ⁻) + NH(X ³ Σ ⁻) + N ₂ (X ¹ Σ) (b)							
Imidogen + Hydrazoic acid							
73 PAU/BAI k _a + k _b . Unreported T assumed to be 298 K.	EX	298	(1.51±0.60)(13)			2	
76 PAU/BAI k _a . Upward revised k.	EX	298	(5.60±0.60)(13)			2	
78 MCD/MIL k _a . HN ₃ photolysis. Gas-chromatography.	EX	298	(5.60±0.54)(13)			2	
80 PIP/KRE k _a . UV-photolysis of HN ₃ at 290 nm. Laser-induced fluorescence. P(Total) = (5-50) torr.	EX	298	1.08(14)			2	
NH(b¹Σ⁺) + NH₃ → products							
Imidogen + Ammonia							
75 ZET/STU	EX	298	2.46(11)			2	1.25

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{NH}(a^1\Delta) + \text{CH}_4 \rightarrow \text{NH}_2(^2A_1) + \text{CH}_3$ (a) $\rightarrow \text{NH}_2(^2B_1) + \text{CH}_3$ (b) $\rightarrow \text{NH}_2\text{CH}_3$ (c)						
Imidogen + Methane 78 MCD/MIL $k_a + k_b + k_c$. HN_3 photolysis. Gas-chromatography. Channel (c) is favored.	EX	298	(7.23±0.60)(12)			2
$\text{NH}(a^1\Delta) + \text{CH}_2=\text{CH}_2 \rightarrow \text{NH}_2(^2A_1) + \text{CH}_2=\text{CH}$ (a) $\rightarrow \text{NH}_2(^2B_1) + \text{CH}_2=\text{CH}$ (b) $\rightarrow \begin{array}{c} \text{H} \\ \text{N} \\ \triangle \end{array}$ (c)						
Imidogen + Ethene 78 MCD/MIL $k_a + k_b + k_c$. HN_3 photolysis. Gas-chromatography. Channel (c) is favored.	EX	298	(2.29±0.24)(13)			2
$\text{NH}(a^1\Delta) + \triangle \rightarrow \text{NH}_2(^2A_1) + \triangle^\bullet$ (a) $\rightarrow \text{NH}_2(^2B_1) + \triangle^\bullet$ (b)						
Imidogen + Cyclopropane 78 MCD/MIL $k_a + k_b$. HN_3 photolysis. Gas-chromatography.	EX	298	(2.17±0.54)(13)			2
$\text{NH}(a^1\Delta) + \text{Cyclohexane} \rightarrow \text{NH}_2(^2A_1) + \text{Cyclohexane}^\bullet$ (a) $\rightarrow \text{NH}_2(^2B_1) + \text{Cyclohexane}^\bullet$ (b)						
Imidogen + Cyclohexane 78 MCD/MIL $k_a + k_b$. HN_3 photolysis. Gas-chromatography.	EX	298	(4.03±0.42)(13)			2
$\text{NH}_2 + \text{O}_2 (+ \text{M}) \rightarrow \text{NH}_2\text{O}_2 (+ \text{M})$ (a) $\rightarrow \text{HNO} + \text{OH} (+ \text{M})$ (b) $\rightarrow \text{NO} + \text{H}_2\text{O} (+ \text{M})$ (c)						
Amidogen + Oxygen molecule 79 PAG/ERI $k_a = k_b = k_c$. Gaseous NH_3 pulse-radiolysis. Upper-limit k's.	ES	300	≤5.0(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 FUJ/MIY1 k_a . Oxidation of NH_3 behind reflected shock-waves. The product is vibrationally excited.	DE	300-1200	3.16(12)	0	7549±252	2
79 FUJ/MIY k_b . Shock-wave induced high-T oxidation of NH_3 . Computer simulation based on a reaction scheme including 13 steps, under the following conditions: $[\text{NH}_3] = [\text{O}_2] = 5\%$. $[\text{Ar}] = 90\%$, and $P = (3.7-7.7)$ atm.	DE	1492-2319	1.26(13)	0	14092	2
77 LES/DEM $k_a + k_b + k_c$. NH_3 flash-photolysis. $P(\text{NH}_3) = 3$ torr. Upper-limit k.	EX	298-500	≤1.81(6)			2
79 CHE/SAR $k_a + k_b + k_c$. NH_3 Flash-photolysis. Laser-Spectroscopy. Upper-limit k. $P < 570$ torr.	EX	298	<9.03(6)			2
79 NAD/SAR4 $k_a + k_b + k_c$. Laser spectroscopy. Upper-limit k.	EX	298	<4.82(7)			2
82 HAC/HOR k_a . M = He. Discharge flow. Laser-induced fluorescence. $P = (1.5-16)$ torr. Limiting low-pressure k. The preexponential factor expressed as: $A(T/298)^{-2.0}$.	EX	295-353	(1.27±0.50)(15)	-2.0	0	3
$\text{NH}_2 + \text{O}_3 \rightarrow \text{HONO} + \text{OH}$ (a)						
$\rightarrow \text{HNO} + \text{HO}_2$ (b)						
$\rightarrow \text{NH}_2\text{O} + \text{O}_2$ (c)						
Amidogen + Ozone						
80 HAC/HOR $k_a + k_b + k_c$. Discharge-flow. $\text{NH}_3 + \text{F} \rightarrow \text{NH}_2 + \text{HF}$.	EX	250-360	1.28(12)	0	638	2
80 KUR/LES ¹⁾	EX	298-380	2.52(12)	0	1258±252	2
80 KUR/LES ¹⁾	EX	298	(3.79±0.60)(10)			2
¹⁾ $k_a + k_b + k_c$. Flash-photolysis. Laser Resonance-fluorescence.						
81 HAC/HOR $k_a + k_b + k_c$. Discharge-flow. $\text{NH}_3 + \text{F} \rightarrow \text{NH}_2 + \text{HF}$.	EX	248-358	(1.21±0.07)(12)	0	710±48	2
80 BUL/BUL k_b . Flash-photolysis of NH_3/O_3 mixtures. Intracavity laser spectroscopy. $P(\text{NH}_3) = 5$ torr.	EX	298	(7.23±1.81)(10)			2
$\text{NH}_2 + \text{H}_2 \rightarrow \text{NH}_3 + \text{H}$						
Amidogen + Hydrogen molecule						
80 DEM/LES Flash-photolysis. Resonance-absorption.	EX	300-520	1.26(12)	0	4278±201	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units factor	k err.
$\text{NH}_2 + \text{NO} \rightarrow [\text{NH}_2\text{NO}] \rightarrow \text{N}_2 + \text{H}_2\text{O}$ (a) $\rightarrow \text{N}_2\text{O} + \text{H}_2$ (b) $\rightarrow \text{N}_2 + \text{H} + \text{OH}$ (c) $\rightarrow \text{N}_2\text{OH} + \text{H}$ (d) $\rightarrow \text{N}_2\text{H} + \text{OH}$ (e)							
Amidogen + Nitrogen oxide (NO)							
72 BED/THO	RL	615-660	5.01(-3)	0	-3221±503	2/2	
k_a . Reaction of NH_3 with NO_2 in a Pyrex vessel. Photo-multiplier. k_{ref} : $\text{NH}_2 + \text{NO}_2 \rightarrow \text{NH} + \text{HONO}$.							
78 SAR/CHE	EX	293	(1.02±0.24)(13)			2	
k_a . Pulse photolysis. Laser Spectroscopy.							
78 ROO/HAN	ES	1700-3000	8.63(9)	0.5	0	2	
k_a . Shock-waves. NH_2 produced by applying incident shock-waves to a NH_3/NO (or $\text{NH}_3/\text{N}_2\text{O}$) mixture in Ar. Emission and IR-Laser-absorption. The pre-exponential factor expressed as: $A(T/298)^{0.5}$.							
79 HAC/SCH2	EX	210-503	7.15(12)	-1.85	0	2	
k_a . Discharge-flow. Resonance-fluorescence. The preexponential factor expressed as: $A(T/298)^{-1.85}$. $P = (0.6-4.0)$ torr.							
79 NAD/SAR4	EX	298	1.02(13)			2	
k_a . Intracavity laser spectroscopy.							
81 ROO/HAN ¹⁾	RL	1680-2850	≈2.3	0	6100	2/2	
$k_a/(k_a + k_b + k_c + k_d + k_e)$. Estimated ratio.							
81 ROO/HAN ¹⁾	EX	1680-2850	7.0(13)	0	14000	2	2.0
k_a . Best data fit.							
¹⁾ NH_2 is produced by applying incident shock-waves to a NH_3/NO (or $\text{NH}_3/\text{N}_2\text{O}$) mixture in Ar.							
81 MOR2	EX	1790	<4.82(12)			2	
$k_a + k_b + k_c + k_d + k_e$. Premixed $\text{H}_2/\text{O}_2/\text{Ar}$ flames. Laser-fluorescence. Upper-limit k. $P = 760$ torr.							
81 ROO/HAN	EX	1680-2850	3.0(13)	0	7900	2	2.0
$k_a + k_b + k_c + k_d + k_e$. M = Ar. NH_2 produced by applying incident shock-waves to a NH_3/NO (or $\text{NH}_3/\text{N}_2\text{O}$) mixture in Ar.							
81 SCH	EX	210-503	(7.15±2.12)(12)	-1.85	0	2	
$k_a + k_b + k_c + k_d + k_e$. Only the initial adduct, and channel (a), detected. Discharge-flow. Resonance-fluorescence. Mass-spectrometry. The preexponential factor expressed as: $A(T/298)^{-1.85}$. $[\text{NO}] = (0.07-1.51) \times 10^{14}$ molec. cm^{-3} . $P = 1$ torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 AND/JAC $k_a + k_b + k_c + k_d + k_e$. Isothermal-flow. NH_2 generated by NH_3 Laser-photolysis. Laser-induced Fluorescence. The most important channel is (e).	EX	295	(1.0±0.3)(13)			2
82 SIL/KOL ¹⁾ The preexponential factor expressed as: $A(T/298)^{-2.30}$.	EX	294-1215	(5.38±0.86)(13)	-2.30	684±60	2
82 SIL/KOL ¹⁾ ¹⁾ $k_a + k_b + k_c + k_d + k_e$. Channels (a), (c) and (e) are most important. Reaction of NH_2 with NO in a high-T fast-flow reactor. NH_2 generated by reacting F with NH_3 . $[\text{NO}] = 4.2 \times 10^{13}$ molec. cm^{-3} . P = (1.0-2.8) torr.	EX	298	5.42(12)			2
82 STI/BRO ²⁾ The preexponential factor expressed as: $A(T/298)^{-1.23}$.	EX	216-480	(1.23±0.40)(13)	-1.23	0	2
82 STI/BRO ²⁾ ²⁾ $k_a + k_b + k_c + k_d + k_e$. Channels (a), (c) and (e) are the most prominent. Flash-photolysis. Laser-induced fluorescence. NH_2 generated by Photolysis of NH_3 in Ar. $P(\text{NH}_3) = (50-250)$ torr. $P(\text{Ar}) = (5-20)$ torr. $P(\text{NO}) < 2.6$ mtorr.	EX	298	(1.26±0.18)(13)			2
$\text{NH}_2 + \text{NO}_2 \rightarrow \text{N}_2\text{O} + \text{H}_2\text{O}$ (a)						
$\rightarrow \text{N}_2 + \text{H}_2\text{O}_2$ (b)						
$\rightarrow \text{NH} + \text{HONO}$ (c)						
Amidogen + Nitrogen oxide (NO_2)						
79 HAC/SCH2 $k_a + k_b$. Discharge-flow. Resonance-fluorescence. Channel (a) predominant. Channel (b) probably less than 5%. P = 1 torr. The preexponential factor expressed as: $A(T/298)^{-3.0}$.	EX	250-503	7.18(12)	-3.0	0	2
79 KUR/LES ¹⁾ The preexponential factor expressed as: $A(T/298)^{-1.3}$.	EX	298-505	1.39(13)	-1.3	0	2
79 KUR/LES ¹⁾ ¹⁾ $k_a + k_b$. Flash-photolysis. Resonance-fluorescence. P(Total) = (3.0-10.5) torr.	EX	298	(1.39±0.12)(13)			2
81 SCH $k_a + k_b$. Discharge-flow. Resonance-fluorescence. Mass-spectrometry. P = (1-16) torr. $[\text{NO}_2] = (0.28-8.43) \times 10^{13}$ molec. cm^{-3} .	EX	250-500	(7.18±1.89)(12)	-3.0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 SCH k _c . Rate constant put on an absolute basis relative to the reaction: NO + NH ₂ → N ₂ + H ₂ O. by using the rate ratio reported in 72 BED/THO. Channel (c) occurs probably at temperatures over 600 K, but not at room temperature.	RN	615-660	1.3(14)	0	2470	2
NH₂ + NH₂ (+ M) → NH₂NH₂ (+ M)						
Amidogen						
71 GOR/MUL Gaseous NH ₃ pulse-radioly	EX	298	6.2(13)			2
73 BAC/YOK	ES	573	(4.7±2.0)(13)			2
77 KHE/SOU ¹⁾ Limiting high-pressure k. No significant T-effect found. P(N ₂) = 1000 torr.	EX	300-500	(1.50±0.75)(13)	0	0	2
77 KHE/SOU ¹⁾ P(N ₂) = 0. (extrapolation to zero-pressure.) E _a = 0 or ±500 cal./mol.	EX	300-500	(8.50±4.25)(14)	0	0	2
79 LOZ/NAD ²⁾ M = Ar, N ₂ . Limiting high-pressure k.	EX	298	(3.61±1.51)(13)			2
79 PAG/ERI Gaseous NH ₃ pulse-radiolysis.	EX	349	1.6(13)			2
71 GEH/HOY M = He. k _{ref} : NH ₂ + NH ₂ → NH + NH ₃	RL	213-473	4.7(6)			3/2
77 KHE/SOU ¹⁾ M = N ₂ . M-efficiencies relative to N ₂ are: 1.0(N ₂), 0.4(Ar), 4.0(NH ₃). No significant T-effect found. At 20 torr. a small negative T-coefficient is observed: -1 < E _a < -0.5 kcal/mol. P < 20 torr.	EX	300-500	(2.55±1.28)(18)	0	0	3
79 LOZ/NAD ²⁾ M = N ₂ . Limiting low-pressure k. M-efficiencies relative to N ₂ are: 1.00(N ₂), 0.42(Ar).	EX	298	(2.50±0.83)(18)			3
¹⁾ Flash-photolysis of NH ₃ .						
²⁾ Intraresonator laser spectroscopy.						
Flash-photolysis.						
P = (10-760) torr.						
NH₂ + NH₂NH₂ → NH₃ + NH₂NH						
Amidogen + Hydrazine						
71 GEH/HOY	EX	300	(3.1±0.4)(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{NH}_2(^2\text{A}_1) + \text{HN}_3(^1\text{A}') \rightarrow \text{NH}_3(^1\text{A}_1) + \text{N}_3(^2\Pi_g)$ (a)						
$\rightarrow \text{NH}_2(^2\text{B}_1) + \text{HN}_3(^1\text{A}')$ (b)						
Amidogen + Hydrazoic acid						
80 PIP/KRE k_a . UV photolysis of HN_3 at 290 nm. Laser-induced fluorescence. P(Tot) = (5-50) torr.	EX	298	5.60(13)			2
78 MCD/MIL $k_a + k_b$. HN_3 photolysis. Gas-chromatography. Channel (b) is predominant.	EX	298	(1.93±0.18)(14)			2
$\text{NH}_2(^2\text{A}_1) + \text{CH}_4 \rightarrow \text{NH}_3(^1\text{A}_1) + \text{CH}_3$ (a)						
$\rightarrow \text{NH}_2(^2\text{B}_1) + \text{CH}_3$ (b)						
Amidogen + Methane						
80 DEM/LES k_a . Flash-photolysis. Resonance-absorption. Tentative k.	ES	300-520	(5.0±2.0)(11)	0	5284±252	2
78 MCD/MIL $k_a + k_b$. HN_3 photolysis. Gas-chromatography. Channel (b) is predominant.	EX	298	(1.81±0.18)(14)			2
$\text{NH}_2 + \text{HCONH}_2 \rightarrow \text{NH}_3 + \text{CONH}_2$						
Amidogen + Formamide						
73 BAC/YOK	ES	573	8.4(9)			2
$\text{NH}_2 + \text{CH}\equiv\text{CH} \rightarrow \text{products}$ (overall)						
Amidogen + Ethyne						
81 SCH Discharge-flow. Mass-spectrometry. Same data given in 70 HAC/SCH ₂ . The preexponential factor expressed as: $A(T/298)^{-2.7}$. P = (0.4-15) torr. [CH≡CH] = (0.15-4.16) × 10 ¹⁶ molec.cm ⁻³ . [NH ₂] ₀ = (0.05-1.20) × 10 ¹³ molec.cm ⁻³ .	EX	210-505	(2.92±0.84)(9)	-2.7	0	2
82 BOS NH_3 flash-photolysis. Laser-induced fluorescence. Limiting high-pressure k. P(Tot) = (5-100) torr.	EX	241-263	(6.69±2.17)(10)	0	1852±100	2
$\text{NH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{products}$ (overall)						
Amidogen + Ethene						
79 KHE/LES ¹⁾	EX	300-500	1.2(11)	0	1988±101	2
79 KHE/LES ¹⁾	EX	300	(1.65±0.25)(8)			2
¹⁾ Flash-photolysis. Laser Resonance-absorption. Supersedes 78 LES/KHE.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 SCH Discharge-flow. Mass-spectrometry. Same data given in 79 HAC/SCH2. [CH ₂ =CH ₂] = (0.04-3.07)x10 ¹⁶ molec.cm ⁻³ . [NH ₂] ₀ = (0.08-1.59)x10 ¹³ molec.cm ⁻³ . P = (0.4-10.5) torr.	EX	295-505	(1.3±0.7)(9)	0	0	2
82 BOS Ammonia Flash-photolysis. Laser-induced fluorescence. P(Tot) = (5-100) torr.	EX	250-365	(2.05±0.07)(10)	0	1318±23	2
NH ₂ (² A ₁) + CH ₂ =CH ₂ → NH ₃ (¹ A ₁) + CH ₂ =CH (a) → NH ₂ (² B ₁) + CH ₂ =CH ₂ (b)						
Amidogen + Ethene						
78 MCD/MIL k _a + k _b . HN ₃ photolysis. Channel (b) predominant.	EX	298	(1.87±0.18)(14)			2
NH ₂ + CH ₃ CH ₂ → CH ₃ CH ₂ NH ₂ (a) → NH ₃ + CH ₂ =CH ₂ (b)						
Amidogen + Ethyl						
82 DEM/LES k _a + k _b . Flash-photolysis. Resonance-Absorption. NH ₂ and CH ₃ CH ₂ generated by flashing NH ₃ in presence of CH ₂ =CH ₂ . Best-fit by simulation. Supersedes 78 LES/DEM.	DE	298	(2.5±0.5)(13)			2
NH ₂ + CH ₃ CH ₃ → NH ₃ + CH ₃ CH ₂						
Amidogen + Ethane						
80 DEM/LES Flash-photolysis. Resonance-absorption.	EX	300-520	3.7(11)	0	3598±141	2
NH ₂ + CH ₂ =C=CH ₂ → products (overall)						
Amidogen + 1,2-Propadiene						
81 SCH Discharge-flow. Mass-spectrometry. Upper-limit k. [CH ₂ =C=CH ₂] = (0.4-1.39)x10 ¹⁶ molec.cm ⁻³ . P = 1 torr. Same data given in 79 HAC/SCH2.	EX	298	≤5.0(8)			2
NH ₂ + CH ₃ CH=CH ₂ → products (overall)						
Amidogen + 1-Propene						
76 LES/SOU	EX	300-500	2.9(11)	0	2164±101	2
76 LES/SOU	EX	300	(2.2±0.3)(8)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 KHE/LES ¹⁾	EX	300-500	2.8(11)	0	2164±101	2	
79 KHE/LES ¹⁾	EX	300	(2.15±0.35)(8)			2	
¹⁾ Flash-photolysis. Resonance-absorption. Supersedes 78 LES/KHE.							
81 SCH	EX	298	≤6.0(8)			2	
Discharge-flow. Resonance-fluorescence. Mass-spectrometry. Upper-limit k. [CH ₃ CH=CH ₂] = (2.10-2.77)×10 ¹⁶ molec.cm ⁻³ . P = 1 torr. Same data given in 79 HAC/SCH2.							
NH₂ + Δ → products (overall)							
Amidogen + Cyclopropane							
81 SCH	EX	250-300	(1.9±0.6)(8)	0	0	2	
Discharge-flow. Mass-spectrometry. [Cyclopropane] = (0.49-7.83)×10 ¹⁶ molec.cm ⁻³ . [NH ₂] ₀ = (0.36-2.41)×10 ¹³ molec.cm ⁻³ . P = (7.5-15) torr.							
$\text{NH}_2(^2\text{A}_1) + \Delta \rightarrow \text{NH}_3 + \dot{\Delta} \quad (\text{a})$ $\rightarrow \text{NH}_2(^1\text{B}_1) + \Delta \quad (\text{b})$							
Amidogen + Cyclopropane							
78 MCD/MIL	EX	298	(1.87±0.18)(14)			2	
k _a + k _b . HN ₃ photolysis. Channel (b) predominant.							
$\text{NH}_2 + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHNH}_2 \quad (\text{a})$ $\rightarrow \text{NH}_3 + \text{CH}_3\text{CH}=\text{CH}_2 \quad (\text{b})$							
Amidogen + Ethyl, 1-methyl-							
82 DEM/LES	DE	298	(2.0±0.4)(13)			2	
k _a + k _b . Flash-photolysis. Resonance-absorption. NH ₂ and (CH ₃) ₂ CH generated by flashing NH ₃ in presence of 1-Propene. Best-fit by simulation. Supersedes 78 LES/DEM.							
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2 \quad (\text{a})$ $\rightarrow \text{NH}_3 + (\text{CH}_3)_2\text{CH} \quad (\text{b})$							
Amidogen + Propane							
80 DEM/LES	EX	300-520	4.5(11)	0	3095±126	2	
k _a + k _b . Flash-photolysis. Resonance-absorption.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NH₂ + CH₂=CHCH=CH₂ → products						
Amidogen + 1,3-Butadiene						
81 SCH ¹⁾	EX	230-360	(3.8±1.3)(11)	0	1140	2
81 SCH ¹⁾	EX	298	(6.7±2.3)(9)			2
¹⁾ Discharge-flow. Mass-spectrometry. [CH ₂ =CHCH=CH ₂] = (0.03-1.20)×10 ¹⁶ molec.cm ⁻³ . [NH ₂] ₀ = (0.22-1.33)×10 ¹³ molec.cm ⁻³ .						
82 HAC/SCH	EX	230-360	3.8(11)	0	1140	2
Discharge-flow. NH ₃ + F → NH ₂ + HF. [1,3-Butadiene] ₀ < 1,0×10 ¹⁶ molec.cm ⁻³ . [NH ₂] ₀ = (0.2-1.2)×10 ¹³ mole.cm ⁻³ . P = (1.5-7.5)						
NH₂ + CH₃CH₂CH=CH₂ → products						
Amidogen + 1-Butene						
79 KHE/LES ¹⁾	EX	300-500	2.8(11)	0	2063±101	2
79 KHE/LES ¹⁾	EX	300	(3.00±0.45)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
NH₂ + cis-CH₃CH=CHCH₃ → products						
Amidogen + 2-Butene, (Z)-						
79 KHE/LES ¹⁾	EX	300-500	3.3(11)	0	2164±101	2
79 KHE/LES ¹⁾	EX	300	(2.55±0.40)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
NH₂ + trans-CH₃CH=CHCH₃ → products						
Amidogen + 2-Butene, (E)-						
79 KHE/LES ¹⁾	EX	300-500	3.5(11)	0	2139±101	2
79 KHE/LES ¹⁾	EX	300	(2.95±0.45)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
NH₂ + (CH₃)₂C=CH₂ → products						
Amidogen + 1-Propene, 2-methyl-						
79 KHE/LES ¹⁾	EX	300-500	4.6(11)	0	2265±101	2
79 KHE/LES ¹⁾	EX	300	(2.55±0.40)(8)			2
¹⁾ Flash-photolysis. Resonance-absorption.						
NH₂ + (CH₃)₃C → (CH₃)₃CNH₂ (a) → NH₃ + (CH₃)₂C=CH₂ (b)						
Amidogen + Ethyl, 1,1-dimethyl-						
82 DEM/LES	ES	298	(2.5±0.5)(13)			2
k _a + k _b . Flash-photolysis. Resonance-absorption. Best-fit by simulation. Supersedes 78 LES/DEM.						



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CHCH}_3$ (b)							
Amidogen + Butane							
80 DEM/LES $k_a + k_b$. Flash-photolysis. Resonance-absorption.	EX	300-520	7.0(11)	0	3070±126	2	
$\text{NH}_2 + (\text{CH}_3)_3\text{CH} \rightarrow \text{NH}_3 + (\text{CH}_3)_3\text{C}$ (a) $\rightarrow \text{NH}_3 + (\text{CH}_3)_2\text{CHCH}_2$ (b)							
Amidogen + Propane, 2-methyl-							
79 KHE/LES ¹⁾	EX	300-500	2.4(11)	0	2516±101	2	
79 KHE/LES ¹⁾	EX	300	(6.2±0.9)(7)			2	
¹⁾ Flash-photolysis. Resonance-absorption.							
80 DEM/LES $k_a + k_b$. Flash-photolysis. Resonance-absorption.	EX	300-520	2.3(11)	0	2466±111	2	
$\text{NH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{NH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3$ (b) $\rightarrow \text{NH}_3 + (\text{CH}_3\text{CH}_2)_2\text{CH}$ (c)							
Amidogen + Pentane							
80 HAC/HOR $k_a + k_b + k_c$. Discharge-flow. $\text{NH}_3 + \text{F} \rightarrow \text{NH}_2 + \text{HF}$.	EX	250-360	3.7(10)	0	1227	2	
$\text{NH}_3 (+ \text{M}) \rightarrow \text{NH}_2 + \text{H} (+ \text{M})$ (a) $\rightarrow \text{NH} + \text{H}_2 (+ \text{M})$ (b)							
Ammonia							
73 GEN/ZHI k_a . M = Ar. Limiting high-pressure k.	EX	2200-2600	6.61(12)	0	49321±2516	1	3.47
72 HAL k_a . M = Ar.	EX	1989-2693	1.0(14)	0	42386	2	
73 GEN/ZHI k_a . M = Ar. Limiting low-pressure k.	EX	2300-3100	5.76(15)	0	38752±2516	2	6.31
77 FIS k_a . M = H ₂ O. Rich NH ₃ /O ₂ /N ₂ flames.	ES	1950-2100	2.7(16)	0	42406	2	
80 ROO/HAN ¹⁾	DE	2200-3450	2.52(16)	0	47200	2	
80 ROO/HAN ¹⁾	DE	2798	1.19(9)			2	
¹⁾ k_a . M = Ar. NH ₃ decomposition behind incident shock-waves. Data-fit. P = (0.14-0.6) atm.							
80 YUM/ASA ²⁾ [NH ₃] ₀ = (0.03-4.8) × 10 ¹⁵ molec.cm ⁻³ . [Ar] = (0.3-5.4) × 10 ¹⁸ molec.cm ⁻³ .	EX	2050-3070	1.38(16)	0	45596	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 YUM/ASA ²⁾ [NH ₃] ₀ = (0.6-4.8)x10 ¹⁴ molec.cm ⁻³ . [Ar] = (0.02-1.2)x10 ¹⁹ molec.cm ⁻³ . 2) k _a . M = Ar. Thermolysis of NH ₃ behind incident shock-waves. Vacuum-UV Absorption-spectroscopy.	EX	1740-3050	1.78(16)	0	46351±1711	2	2.14
80 ROO/HAN ³⁾ k _b .	DE	2798	3.4(6)			2	
80 ROO/HAN ³⁾ k _b /k _a .	RL	2798	≤1.0(-2)			2/2	
3) NH ₃ decomposition behind incident shock-waves. Rate constant and rate ratio determined by computer simulation. P = (0.14-0.6) atm.							
73 VOM1 k _a + k _b . M = Ne.	EX	2300-3200	2.51(14)	0	33216±2013	2	2.0
72 HAL k _a + k _b . M = Ar. Overall decomposition.	EX	1989-2693	4.12(12)	0	41983	2	
79 DOV/NIP k _a + k _b . Pyrolysis behind reflected shock-waves. M = (88.9-99.7)% Kr + (0.16-5.0)% Ar. Data-fit.	EX	2500-3000	1.2(16)	0	45798	2	2.0
81 HOL/WAG ⁴⁾ k _a + k _b . M = Ar. Limiting low-pressure k.	EX	200-330	4.0(16)	0	47272	2	
81 HOL/WAG ⁴⁾ k _a + k _b . M = Ar. Extrapolated limiting high-pressure k.	EX	2200-3300	5.5(15)	0	54250	1	
4) Thermolysis of NH ₃ behind shock-waves. Total density = 5.4x10 ¹⁷ -1.2x10 ²⁰ molec.cm ⁻³ .							
NH₃ + HONO → products							
Ammonia + Nitrous acid							
78 KAI/JAP2 Discharge-flow. Upper-limit k.	EX	300	≤9.03(6)			2	
NH₃ + CH₂=CHCN → NH₂CH₂CH₂CN							
Ammonia + 2-Propenenitrile (Acrylonitrile) → Propanenitrile, 3-amino- (β-Aminopropionitrile)							
82 SAI/MIC Reaction in an Autoclave.	EX	303-408	6.55(13)	0	9109	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
NH=NH → products						
Diazene						
73 WIL/BAC Decomposition in gas phase at 295 K. The only products observed: N ₂ , H ₂ , and NH ₂ NH ₂ . Ammonia not observed, but cannot be ruled out.	EX	295	(3.8±0.5)(-3)			1
cis-NH=NH + CH₂=CHCH=CH₂ → N₂ + CH₃CH₂CH=CH₂ Diazene, (Z)- + 1,3-Butadiene						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(6.5±0.7)(-2)			2/2
cis-NH=NH + cis-CH₃CH=CHCH₃ → N₂ + CH₃CH₂CH₂CH₃ Diazene, (Z)- + 2-Butene, (Z)-						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(1.1±0.1)(-1)			2/2
cis-NH=NH + trans-CH₃CH=CHCH₃ → N₂ + CH₃CH₂CH₂CH₃ Diazene, (Z)- + 2-Butene, (E)-						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(3.3±0.3)(-1)			2/2
cis-NH=NH +  → N₂ + 						
Diazene, (Z)- + 1,3-Cyclohexadiene						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(5.0±0.2)(-2)			2/2
cis-NH=NH + (CH₃)₂C=C(CH₃)₂ → N₂ + (CH₃)₂CHCH(CH₃)₂ Diazene, (Z)- + 2-Butene, 2,3-dimethyl-						
74 VID/WIL k _{ref} : cis-NH=NH + CH ₂ =CH ₂ → N ₂ + CH ₃ CH ₃ Estimated ratio.	RL	373	(2.0±0.1)(-2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
trans-NH=NH → cis-NH=NH (a)						
trans-NH=NH + cis-NH=NH → NH₂NH₂ + N₂ (b)						
→ trans-NH=NH + N₂ + H₂ (c)						
Diazene, (E)-						
77 WIL/BAC	EX	296-433	3.0	0	2114	1
$k_a + k_b + k_c$.						
74 VID/WIL	ES	373	~1.0(-2)			1
k_a .						
77 WIL/BAC	ES	296-433	1.8	0	2114	1
k_a . Determined from the above mechanism.						
74 VID/WIL	RL	373	(6.0±2.0)			2/2
k_b/k_{ref} . Estimated ratio.						
k_{ref} :						
$cis-NH=NH + CH_2=CH_2 → N_2 + CH_3CH_3$						
77 WIL/BAC	RL	296-433	2.33			2/2
k_b/k_c . Determined from the above mechanism.						
trans-ND=ND → cis-ND=ND (a)						
trans-ND=ND + cis-ND=ND → ND₂ND₂ + N₂ (b)						
→ trans-ND=ND + N₂ + D₂ (c)						
Diazene-d ₂ , (E)-						
77 WIL/BAC	EX	296-433	2.0	0	2214	1
$k_a + k_b + k_c$.						
77 WIL/BAC	ES	296-433	1.0	0	2214	1
k_a . Determined from the above mechanism.						
77 WIL/BAC	RL	296-433	4.9(1)			2/2
k_b/k_c . Determined from the above mechanism.						
NH₂NH + NH₂NH → NH₃ + NH₃ + N₂						
Hydrazyl						
79 PAG/ERI	EX	349	1.0(14)			2
Gaseous NH ₃ pulse-radiolysis.						
NH₂NH₂ (+ M) → NH₂ + NH₂ (+ M)						
Hydrazine						
74 GEN/ZHI	EX	1100-1400	3.98(13)	0	26673±1007	1 2.51
M = Ar. Limiting high-pressure k.						
HN₃ (+ M) → NH(a¹Δ) + N₂(¹Σ_g⁺) (+ M) (a)						
→ NH(³Σ⁻) + N₂(¹Σ_g⁺) (+ M) (b)						
Hydrazoic acid						
72 ZAS/KOG	EX	1045-1450	1.78(11)	0	20131	1
$k_a + k_b$. M = Ar. Channel (a) is predominant.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 KAJ/YAM $k_a + k_b$. M = Ar. HN_3 Thermolysis. Channel (b) is predominant in this T-range. P(Ar) = (600-2200) torr.	EX	1200-1350	7.59(14)	0	18218±805	2	1.9
82 DUP/PAI ¹⁾	EX	1250-1400	5.5(13)	0	14000	2	
82 DUP/PAI ¹⁾	EX	1450-2000	2.2(12)	0	9750	2	
¹⁾ $k_a + k_b$. M = Ar. Thermolysis of HN_3 in Ar behind incident shock-waves. 0.5% HN_3 . (98-99.5)% Ar. Channel (a) is predominant.							
79 KAJ/YAM k_b . NH_3 pyrolysis. P(Ar) = (600-2200) torr.	EX	1200-1350	7.59(13)	0	15702±1007	2	2.24
$\text{HNO} + \text{HNO} \rightarrow \text{H}_2\text{O} + \text{N}_2\text{O}$ (a)							
$\rightarrow \text{H}_2\text{O}_2 + \text{N}_2$ (b)							
Nitrosyl hydride							
73 WIE/HEI k_a/k_b . T-independent k.	RL	298-423	5.1(1)	0	0		2/2
75 CAL/CAR k_a . Flash Photolysis of H_2/NO mixtures. HNO absorption at 207.3 nm.	EX	295	(3.22±1.08)(9)			2	
81 CHE/NAD k_a . $\text{CH}_3\text{CHO}/\text{HCHO}/\text{NO}$ flash-photolysis. Intracavity Laser-spectroscopy. P(NO) = (6-20) torr. P(HCHO) = 7 torr. P(CH_3CHO) = 12.2 torr.	EX	298	(9.03±4.82)(8)			2	
$\text{DNO} + \text{DNO} \rightarrow \text{D}_2\text{O} + \text{N}_2\text{O}$							
Nitrosyl hydride-d							
75 CAL/CAR D_2/NO flash-photolysis. 206.4 nm. DNO absorption.	EX	295	(1.31±0.48)(9)			2	
$\text{HONO} (+ \text{M}) \rightarrow \text{OH} + \text{NO} (+ \text{M})$							
Nitrous acid							
76 FIF M = Ar. Limiting high-pressure k.	EX	1000-1400	≥5.5(12)	0	24157	1	
$\text{HONO}^\ddagger \rightarrow \text{OH} + \text{NO}$							
Nitrous acid							
76 OVE/PAR M = H_2O , CF_2 , SF_6 , N_2 , Ar, or He. HONO^\ddagger formed by OH + NO.	EX	295	(1.18±0.186)(9)			1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
HONO + O₃ → HONO₂ + O₂						
Nitrous acid + Ozone						
77 KAI/JAP ¹⁾	EX	226	≤3.01(5)			2
77 KAI/JAP ¹⁾	EX	300	≤6.02(4)			2
¹⁾ Upper limit k's. P(Tot) = (20-30) torr.						
79 STR/WEL	EX	296	≤(2.71±1.81)(5)			2
Upper-limit k.						
HONO + HONO → NO + HO₂ + H₂O						
Nitrous acid						
75 ENG/COR	RN	298	5.6(6)			2
75 ENG/COR	DE	298-323	(1.10±0.21)(13)	0	4320±62	2
A and B recalculated from the reported data. Optimization. k ₁ = k ₋₁ K.						
76 CHA/NOR	EX	296	(5.71±1.63)(5)			2
HONO + HONO₂ → NO₂ + NO₂ + H₂O						
Nitrous acid + Nitric acid						
74 ENG/COR	EX	298	(5.85±0.31)(6)			2
74 ENG/COR	EX	298-323	(3.71±0.48)(12)	0	3987±41	2
A and B recalculated from the reported data.						
77 KAI/WU	EX	300	(9.34±1.81)(6)			2
79 STR/WEL	EX	296	6.63(6)			2
HONO₂ (+ M) → OH + NO₂ (+ M)						
Nitric acid						
74 GLA/TRO1 ¹⁾	EX	900-1200	≈2.0	0	24660	1
Extrapolated limiting high-pressure k.						
74 GLA/TRO1 ¹⁾	RN	295-1200	1.26(15)	0	24006	1 1.58
Limiting high-pressure k over extended T-range.						
73 GER/DEM	EX	1013-1170	1.39(15)	0	16105±906	2 2.00
M = He.						
74 GLA/TRO1 ¹⁾	EX	900-1200	≈2.2(17)	0	20130	2
Extrapolated, Limiting low-presssure k. Concentration-dependent Arrhenius expression = k/[Ar].						
74 GLA/TRO1 ¹⁾	RN	295-1200	1.10(20)	-1.98	24006	2 1.58
Extended T-range, limiting low-pressure k. Concentration-dependent Arrhenius expression = k/[Ar]. The preexponential factor expressed as: A(T/298) ^{-1.98} .						
¹⁾ M = Ar.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 BAS/KOG	EX	863-1173	6.0(14)	0	15148±1596	2	4.68
79 GER/DEM	EX	1050-1200	1.69(15)	0	16105±906	2	2.0
M = He.							
M-efficiencies relative to He are:							
1.0(He), 0.77(Ar), 1.1(N ₂). P = (2-5) torr.							
HO₂NO₂ (+ M) → HO₂ + NO₂ (+ M) (a)							
→ HONO + O ₂ (+ M) (b)							
Peroxynitric acid							
77 GRA/WIN ¹⁾	EX	254-283	1.4(14)	0	10418±252	1	1.1
77 COX/DER ¹⁾	EX	300-328	1.26(16)	0	11700±110	1	39.8
78 GRA/WIN ¹⁾	EX	278	~1.8(-2)			1	
M = N ₂ . Limiting high-pressure k.							
77 SIM/HEI ¹⁾	RN	245-328	6.0(17)	0	13085	1	
78 SIM/HEI ^{1) 2)}	RN	245-328	6.31(17)	0	13085±2516	1	
Δlogk = 3.5.							
¹⁾ k _a .							
78 SIM/HEI ²⁾	RL	245-328	3.0(9)	0	5788	1/1	
k _a /k _b .							
78 SIM/HEI ²⁾	EX	245-328	1.0(8)	0	7046±755	1	10.0
k _b .							
²⁾ N ₂ O/H ₂ /O ₂ /NO photolysis.							
78 GRA/WIN	EX	261-295	3.13(18)	0	10015±252	2	
k _a . M = N ₂ .							
M-efficiencies relative to N ₂ are:							
1.00(N ₂), 0.83(O ₂). Limiting low-pressure k.							
NH₂O → NHOH							
Nitroxide							
80 BUL/BUL	EX	298	(1.3±0.1)(3)			1	
NH₂O + O₃ → NH₂ + O₂ + O₂							
Nitroxide + Ozone							
80 BUL/BUL	EX	298	(1.2±0.9)(10)			2	
NH₂O₂[†] → NH₂ + O₂ (a)							
→ HNO + OH (b)							
Aminodioxy							
81 FUJ/MIY1 ¹⁾	DE	300-2200	(1.0±0.3)(10)	0	0	1	
k _a .							
81 FUJ/MIY1 ¹⁾	DE	300-2200	(1.3±0.3)(10)	0	0	1	
k _b .							
¹⁾ Oxidation of NH ₃ behind reflected shock-waves.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C + O₂ → CO + O						
Carbon atom + Oxygen molecule						
71 HUS/KIR3 Vacuum-UV Time-Resolved Resonance Radiation.	EX	300	(1.99±0.90)(13)			2
75 HUS/YOU	EX	300	(1.57±0.18)(13)			2
C(2¹D₂) (+ M) → products						
Carbon atom						
71 HUS/KIR2 M = CO. M-efficiencies relative to CO are: 1.00(CO), 2.31(CO ₂), 2.94(NO), 8.75(N ₂ O), 8.75(N ₂ O), 13.13(CH ₄), ~1.63(O ₂), ~1.06(H ₂ O), ~23.13(CH ₂ =CH ₂).	EX	300	(9.64±3.61)(12)			2
C(2¹D₂) + H₂ → CH + H						
Carbon atom + Hydrogen molecule						
71 HUS/KIR1	EX	300	(1.57±0.18)(14)			2
C + H₂ (+ M) → CH₂ (+ M)						
Carbon atom + Hydrogen molecule						
71 HUS/KIR3 M = He. Vacuum-UV Time-Resolved Resonance Radiation.	EX	300	(2.58±0.91)(16)			3
75 HUS/YOU M = He.	EX	300	(2.5±0.44)(16)			3
C + H₂O → CO + N₂ (a) → HCHO (b)						
Carbon atom + Water						
71 HUS/KIR3 k _a + k _b . Vacuum-UV Time-Resolved Resonance Radiation. Upper-limit k.	EX	300	≤2.17(11)			2
75 HUS/YOU k _a + k _b . Upper-limit k.	EX	300	<6.02(11)			2
C + N₂ (+ M) → CN₂ (+ M)						
Carbon atom + Nitrogen molecule						
71 HUS/KIR3 M = Ar. Vacuum-UV Time-Resolved Resonance Radiation.	EX	300	(1.12±0.54)(15)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C + NO → CN + O						
Carbon atom + Nitrogen oxide (NO)						
71 HUS/KIR3 Time-Resolved Resonance Radiation.	EX	300	(4.40±1.33)(13)			2
75 HUS/YOU	EX	300	(2.89±0.49)(13)			2
C + N₂O → CO + N₂ (a) → CN + NO (b)						
Carbon atom + Nitrogen oxide (N ₂ O)						
71 HUS/KIR3 k _a + k _b . Time-Resolved Resonance Radiation.	EX	300	(1.51±0.96)(13)			2
75 HUS/YOU k _a + k _b .	EX	300	(7.83±1.81)(12)			2
C + C (+ M) → C₂ (+ M)						
Carbon atom						
76 SLA M = Ar. Based on reverse reaction measurements. The preexponential factor expressed as: A(T/298) ^{-1.6} .	ES	5000-6000	(1.98±1.10)(17)	-1.6	0	3
C + CO (+ M) → C₂O (+ M)						
Carbon atom + Carbon monoxide						
71 HUS/KIR3 M = He. Vacuum UV Time-Resolved Resonance Radiation.	EX	300	(2.29±0.98)(16)			3
C + CO₂ → CO + CO						
Carbon atom + Carbon dioxide						
71 HUS/KIR3 Time-Resolved Resonance-Radiation. Upper-limit k.	EX	300	<6.02(9)			2
75 HUS/YOU Upper-limit k.	EX	300	<6.02(8)			2
C + CH₂ → H₂ + C₂(d³Π_g)						
Carbon atom + Methylene						
82 GRE/HOM2 Reaction of the CH≡CH/CH/O/H system, diluted in N ₂ /He carrier gas. Discharge-flow. Resonance-fluorescence. O atoms generated by reacting N with NO. P = 2 torr.	EX	298	≈7.0(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C + CH₄ → CH₂=CH₂						
Carbon atom + Methane						
71 HUS/KIR3 Time-Resolved Resonance-Radiation. Upper-limit k.	EX	300	<1.20(9)			2
C + CN → C₂ + N						
Carbon atom + Cyanogen						
76 SLA	ES	5000-8000	(3.0±1.5)(14)	0	18118	2
C + O=C=C=O → products						
Carbon atom + 1,2-Propadiene-1,3-dione						
75 HUS/YOU	EX	300	(1.08±0.12)(14)			2
C(¹S₀) + O=C=C=O → products						
Carbon atom + 1,2-Propadiene-1,3-dione						
74 HUS/KIR	EX	300	6.02(13)			2
CO + O₂ → CO₂ + O						
Carbon monoxide + Oxygen molecule						
71 BRA/BEL1	ES	1300-1900	1.6(13)	0	20634	2 3.47
71 DEA/KIS Shock-waves. Best-fit to experimental data.	DE	1750-2575	1.20(13)	0	30196	2
74 RAW/GAR1 Shock-waves.	EX	1500-2500	1.2(11)	0	17614	2
76 WEI	EX	2500-2900	2.5(13)	0	24157	2
CO + O₃ → products						
Carbon monoxide + Ozone						
72 ARI/WAR Upper-limit k. Possible products: CO ₂ + O ₂ .	EX	296	≤2.41(-1)			3
73 STE/NIK2 Upper-limit k.	EX	298	≤6.02(2)			2
CO + SO₂(³B₁) → CO₂ + SO						
Carbon monoxide + Sulfur dioxide						
77 SU/CAL Photolysis of SO ₂ /CO mixtures.	EX	298	2.60(9)			2
CO + NO₂ → CO₂ + NO						
Carbon monoxide + Nitrogen oxide (NO ₂)						
76 MIL	EX	950-1500	3.24(13)	0	16105±654	2 1.78
77 FRE/PAL	EX	1309-1946	2.19(13)	0	14696±805	2 1.66

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 FRE/PAL Best fit. Preferred k.	SE	298-2000	8.9(13)	0	17011	2	2.0
79 MIL/ADA Single-pulse shock-tube.	EX	950-1500	3.24(13)	0	16105±654	2	1.78
80 PAL/FRE Incident shock-waves. P = (10-70) torr.	EX	950-1950	8.91(13)	0	17011	2	
CO + NO₂(²B₂) → CO₂ + NO							
Carbon monoxide + Nitrogen oxide (NO ₂) ^e							
76 HER/MAR At (506±1) nm.	EX	298	7.23(8)			2	
76 HER/MAR At 750 nm.	EX	298	1.33(8)			2	
78 HER/MAR Laser-induced fluorescence. At 488 nm.	EX	298	(1.93±0.72)(9)			2	
CO + N₂O → CO₂ + N₂							
Carbon monoxide + Nitrogen oxide (N ₂ O)							
73 MIL/MAT	EX	1169-1655	2.09(11)	0	8707±1158	2	2.29
76 MIL	EX	1169-1655	7.08(11)	0	10569±1057	2	2.19
79 ZAS/LOS ¹⁾ In 76% Ar.	EX	1700-2500	2.75(15)	0	25164±604	2	5.75
79 ZAS/LOS ¹⁾ In 97% Ar.	EX	1500-1900	7.08(14)	0	26673±2013	2	2.0
¹⁾ Exchange reaction behind reflected shock-waves.							
CO₂ (+ M) → CO + O (+ M)							
Carbon dioxide							
74 WAG/ZAB M = Ar. Limiting high-pressure k.	EX	2740-3700	9.0(12)	0	65274	1	
73 DEA M = Ar.	EX	3700-5600	6.31(13)	0	42637±926	2	1.23
74 HAR/VAS M = Ar. In Aluminum shock-tubes. Low P.	EX	3400-4400	2.7(14)	0	53347	2	
74 HAR/VAS M = Ar. In Brass shock-tubes. Low P.	EX	2700-4300	4.7(14)	0	52843	2	
74 KIE M = Kr. Shock waves.	EX	3600-6503	3.89(14)	0	53951±503	2	
74 WAG/ZAB M = Ar. Concentration-dependent Arrhenius expression = k[Ar]. Limiting low-pressure k.	EX	3000-4561	5.1(14)	0	55561	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
76 EBR/SAN The preexponential factor expressed as: $A(T/298)^{0.5}$.	EX	2500-7000	1.29(14)	0.5	52340±1258	2
CO₂ + C₂O → products						
Carbon dioxide + Carbon oxide (C ₂ O)						
80 DON/PIT Laser photodissociation of C ₃ O ₂ at 266 nm. Dye-laser induced fluorescence. Upper-limit k.	EX	298	<6.02(9)			2
CH + O₂ → CO + OH(A²Σ⁺) (a)						
→ CO ₂ + H (b)						
→ CHO + O (c)						
→ CO + O + H (d)						
Methylidyne + Oxygen molecule						
79 MES/SAD k _a . Laser-induced fluorescence.	EX	298	(1.99±0.24)(13)			2
82 GRE/HOM1 Ethyne/O/H reaction in He/N ₂ . Discharge-flow. Resonance-fluorescence. Best-fit. O atoms generated reacting N with NO. H atoms produced by a discharge of a H ₂ /He mixture. P = 2 torr.	EX	298	4.8(10)			2
71 BOS/PER k _a + k _b + k _c + k _d . Upper-limit k.	EX	298	≤2.4(13)			2
81 BUT/FLE k _a + k _b + k _c + k _d . Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. Same data in 80 BUT/FLE. P(Total) = 100 torr.	EX	298	(3.55±0.48)(13)			2
82 BER/FLE2 k _a + k _b + k _c + k _d . M = Ar. Laser-photolysis/LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. and monitored by LiF at 430 nm.	EX	297-676	(3.25±0.60)(13)	0	0	2
CH + H₂ → products						
Methylidyne + Hydrogen molecule						
71 BOS/PER	EX	298	(1.05±0.12)(13)			2
79 BUT/GOS Multiphoton photodissociation of CHBr ₃ . Laser-Induced Multiphoton Fluorescence. P ~ 2mtorr.	EX	298	(1.39±0.30)(13)			2
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-Induced Fluorescence. Same data in 80 BUT/FLE. P(Total) = 100 torr.	EX	298	(1.57±0.30)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH + H₂O → products						
Methylidyne + Water						
71 BOS/PER	EX	298	(2.7±0.5)(13)			2
CH + N₂ (+ M) → CHN₂ (+ M) (a)						
→ [HCN ₂] → HCN + N (+ M) (b)						
Methylidyne + Nitrogen molecule						
71 BOS/PER	EX	298	(6.1±1.0)(11)			2
k _a .						
79 BUT/GOS	EX	298	(4.64±1.20)(11)			2
k _a . CHBr ₃ Multiphoton dissociation.						
Laser-induced Fluorescence. P = 2 torr.						
81 BUT/FLE	EX	298	(5.60±0.60)(11)			2
k _a . CHBr ₃ Multiphoton dissociation at 193 nm.						
Laser-induced fluorescence.						
P(CHBr ₃) = (5-50) torr.						
P(Total) = 100 torr.						
Same data given in 80 BUT/FLE.						
82 WAG/CAR ¹)	ES	298	(3.79±0.78)(11)			2
k _b . Limiting high-pressure k.						
82 WAG/CAR ¹)	ES	298	(9.43±0.11)(16)			3
k _b . Limiting low-pressure k.						
¹) Laser-induced fluorescence.						
CH generated by Multiphoton dissociation						
of CH ₃ CN, or CH ₃ NH ₂ in Ar.						
CH + NO → CO + NH (a)						
→ CN + OH (b)						
→ HCN + O (c)						
→ HCO + N (d)						
→ CNO + H (e)						
Methylidyne + Nitrogen oxide (NO)						
82 LE	ES	2700	6.0(14)			2
k _a . Premixed fuel-rich Ethyne/NO flames,						
at 250-600 nm.						
P = 80 torr.						
81 BUT/FLE	EX	298	(1.75±0.42)(14)			2
k _a + k _b + k _c + k _d + k _e .						
CHBr ₃ Multiphoton dissociation at 193 nm.						
Laser-induced-fluorescence.						
P(CHBr ₃) = (5-50) torr.						
P(Total) = 100 torr.						
Same data given in 80 BUT/FLE.						



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
82 BER/FLE2 $k_a + k_b + k_c + k_d + k_e$. M = Ar. Laser-photolysis/LIF. CH generated by CHBr_3 Multiphoton dissociation at 266 nm. P(Total) 100 torr. (Ar).	EX	297-676	(1.14±0.18)(14)	0	0	2	
82 WAG/CAR $k_a + k_b + k_c + k_d + k_e$. Laser-induced Fluorescence. CH generated by IR-Multiphoton dissociation of CH_3NH_2 , or Cyclopropane in Ar. P(Ar) = 5 torr.	EX	298	(1.20±0.18)(13)			2	
CH + NO₂ → NH + CO₂ (a) → CO + HNO (b) → CHO + NO (c) → HCN + O ₂ (d) → CO + NO + H (e) → NCO + OH (f)							
Methylidyne + Nitrogen oxide (NO ₂)							
82 WAG/CAR $k_a + k_b + k_c + k_d + k_e + k_f$. Laser-induced Fluorescence. CH generated by IR-Multiphoton dissociation of CH_3CN , or CH_3NH_2 , or Cyclopropane in Ar. P(Ar) = 5 torr.	EX	298	(1.00±0.06)(13)			2	
CH + N₂O → products Methylidyne + Nitrogen oxide N ₂ O							
82 WAG/CAR Laser-induced fluorescence. CH generated by IR-Multiphoton dissociation of CH_3NH_2 , or Cyclopropane in Ar. P(Ar) = 20 torr.	EX	298	(4.70±0.84)(13)			2	
CH + NH₃ → products Methylidyne + Ammonia							
71 BOS/PER	EX	298	5.9(10)			2	1.17
CH + CO → products Methylidyne + Carbon monoxide							
71 BOS/PER	EX	298	2.9(12)			2	
81 BUT/FLE 193 nm. CHBr_3 Multiphoton dissociation at 193 nm. at 193 nm. Laser induced fluorescence. Same data given in 80 BUT/FLE. P(CHBr_3) = (5-50) mtorr. P(Total) = 100 torr.	EX	298	(1.26±0.18)(13)			2	



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 BER/FLE2 Reaction of CH with CO in Ar. Laser-photolysis/ LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. P(Total) = 100 torr. (Ar)	EX	297-676	(2.77±0.60)(11)	0	-861±101	2
CH + CO₂ → products						
Methylidyne + Carbon dioxide						
81 BUT/FLE CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence. Same data given in 80 BUT/FLE. P(Total) 100 torr. P(CHBr ₃) = (5-50) mtorr.	EX	298	(1.14±0.24)(12)			2
82 BER/FLE2 M = Ar. Laser-photolysis/LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. P(Total) = 100 torr. (Ar)	EX	297-676	(3.43±0.54)(12)	0	345±53	2
CH + CH₂ → H₂ + CH=C*						
Methylidyne + Methylene						
82 GRE/HOM2 Reaction of the CH=CH/O/H in N ₂ /He. Discharge-flow. Resonance-fluorescence. Lower-limit k. P = 2 torr.	EX	298	≥1.0(14)			2
CH + CH₄ → products						
Methylidyne + Methane						
71 BOS/PER	EX	298	(2.01±0.05)(13)			2
79 BUT/GOS CHBr ₃ Multiphoton photodissociation. Laser-induced fluorescence. Superseded by 81 BUT/FLE. P ~ 2 mtorr.	EX	298	(1.81±0.60)(14)			2
81 BUT/FLE CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence. P(CHBr ₃) = (5-50) mtorr. P(Total) = 100 torr. Same data given in 80 BUT/FLE.	EX	298	(6.02±1.81)(13)			2
CH + CH=CH → products						
Methylidyne + Ethyne						
71 BOS/PER	EX	298	4.5(13)			2 1.2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
80 FLE/FUJ CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence.	EX	298	(8.42±2.71)(13)			2
81 BUT/FLE CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence. P(CHBr ₃) = (5-50) mtorr. P(Total) = 100 torr.	EX	298	(1.33±0.24)(14)			2
82 BER/FLE1 M = Ar. Laser-photolysis/LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. Before forming the products, CH adds to the triple bond, giving the intermediate:  P(Total) = 100 torr. (Ar)	EX	160-652	(2.10±0.25)(14)	0	-61±36	2
CH + CH ₂ =CH ₂ →  → CH ₂ -CHCH ₂ (a) → any other products (b)						
Methyldiyne + Ethene						
82 BER/FLE1 k _a . M = Ar. Laser-photolysis/LIF. CH generated by CHBr ₃ Multiphoton dissociation at 266 nm. P(Total) = 100 torr. (Ar)	EX	171-657	(1.34±0.16)(14)	0	-173±35	2
71 BOS/PER k _{overall} .	EX	298	(6.9±0.6)(13)			2
80 FLE/FUJ k _{overall} . CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence.	EX	298	(1.54±0.08)(14)			2
81 BUT/FLE k _{overall} . CHBr ₃ Multiphoton dissociation at 193 nm. Laser-induced fluorescence. P(CHBr ₃) = (5-50) mtorr. P(Total) = 100 torr.	EX	298	(1.26±0.48)(14)			2
CH + CH ₃ CH ₃ → products						
Methyldiyne + Ethane						
81 BUT/FLE CHBr ₃ Multiphoton dissociation at 193 nm. Laser induced fluorescence. Same data given in 80 BUT/FLE. P(Total) = 100 torr. P(CHBr ₃) = (5-50) mtorr.	EX	298	(2.41±0.6)(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH + CH₃C≡CH → products						
Methylidyne + 1-Propyne						
80 FLE/FUJ Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence.	EX	298	(2.64±0.51)(14)			2
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. P(Total) = 100 torr.	EX	298	(2.77±0.90)(14)			2
CH +  → products						
Methylidyne + Cyclopropane						
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. P(Total) = 100 torr.	EX	298	(1.44±0.42)(14)			2
CH + CH₃CH₂CH₃ → products						
Methylidyne + Propane						
71 BOS/PER	EX	298	8.2(13)			2 1.2
CH + CH₃CH₂CH₂CH₃ → products						
Methylidyne + Butane						
71 BOS/PER	EX	298	(7.8±0.7)(13)			2
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. P(Total) = 100 torr. Same data given in 80 BUT/FLE.	EX	298	(3.49±0.30)(14)			2
CH +  → products						
Methylidyne + Cyclohexane						
81 BUT/FLE Multiphoton dissociation of CHBr ₃ at 193 nm. Laser-induced fluorescence. P(Total) = 100 torr.	EX	298	(2.77±1.14)(14)			2
CH₂(X³B₁) + O₂ → products						
Methylene + Oxygen molecule						
73 JON/BAY2 k _{ref} : CH ₂ + O → CO + H + H.	RL	296	(9.5±3.0)(-2)			2/2
73 PEE/MAH2	ES	1200-1600	1.0(14)	0	1860	2
74 LAU/BAS	EX	298	(9.03±0.60)(11)			2
M = He. Limiting high-pressure k.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 PEE/VIN1	ES	2000	≈1.2(13)			2	
75 PEE/VIN2	RL	1500-2200	≈3.0			2/2	
k _{ref} : OH + CH ₃ → H ₂ O + CH ₂ . Average ratio.							
75 PEE/VIN2	RN	1500-2200	≈1.2(13)	0	0	2	
NH ₄ /O ₂ and CH ₂ =CH ₂ /O ₂ flames, diluted in Ar. k determined relative to reaction: OH + CH ₃ → H ₂ O + CH ₂							
77 PIL/ROB	ES	298	7.23(11)			2	
79 VIN/DEB1 ¹⁾	EX	295-600	1.33(13)	0	755±151	2	1.55
79 VIN/DEB2 ¹⁾	EX	295	(1.02±0.24)(12)			2	
¹⁾ CH=CH oxidation. Fast-flow. P(Total) 2.2 torr.							
CH ₂ (a ¹ A ₁) + O ₂ → products Methylene + Oxygen molecule							
74 LAU/BAS	EX	298	<1.81(13)			2	
M = He. Limiting high-pressure, upper-limit k.							
CH ₂ (X ³ B ₁) + H ₂ → CH ₃ + H Methylene + Hydrogen molecule							
77 PIL/ROB	ES	298	<3.01(9)			2	
Upper-limit k.							
CH ₂ (a ¹ B ₁) + H ₂ → CH ₃ + H Methylene + Hydrogen molecule							
77 PIL/ROB	ES	298	1.20(13)			2	
CH ₂ (¹ A ₁) + H ₂ O → CH ₃ OH Methylene + Water							
81 HAT/BAN	RN	298	≈1.81(12)			2	
Diazomethane Photolysis in air, or N ₂ , in presence of Water. P(Diazomethane) ~ 9 mtorr. P(air, or N ₂) = 760 torr. P(H ₂ O) = (0-4) torr. k estimated relative to the reaction: CH ₂ (¹ A ₁) + CH ₂ N=N → CH ₂ =CH ₂ + N ₂ .							
CH ₂ (X ³ B ₁) + N ₂ → HCN + NH Methylene + Nitrogen molecule							
78 LAU/BAS	EX	300	≤6.02(7)			2	
Flash-photolysis of CH ₂ CO/N ₂ and CH ₂ N ₂ /N ₂ systems. Upper-limit k.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₂(X³B₁) + NO → CH₂NO → products						
Methylene + Nitrogen oxide (NO)						
74 LAU/BAS M = He. Limiting high-pressure k.	EX	298	(9.64±0.60)(12)			2
77 PIL/ROB	ES	298	6.02(12)			2
79 VIN/DEB1 CH=CH oxidation. Fast-flow. P(Total) = 2.2 torr.	EX	295-600	(1.39±0.83)(12)	0	-554±201	2
CH₂(a¹A₁) + NO → products						
Methylene + Nitrogen oxide (NO)						
74 LAU/BAS M = He. Limiting high-pressure, upper-limit k.	EX	298	<2.41(13)			2
CH₂(X³B₁) + CO → CH=CH + O (a) → any other products (b)						
Methylene + Carbon monoxide						
81 TSU/HAS k _a . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ mixtures behind reflected shock-waves.	ES	1200-1800	1.34(13)	0	26943	2
74 LAU/BAS k _{overall} . Limiting high-pressure, upper-limit k.	EX	298	6.02(8)			2
CH₂(a¹A₁) + CO → products						
Methylene + Carbon monoxide						
74 LAU/BAS M = He. Limiting high-pressure, upper-limit k.	EX	298	<5.42(12)			2
CH₂(X³B₁) + CO₂ → HCHO + O₂						
Methylene + Carbon dioxide						
77 LAU/BAS	EX	298	2.3(10)			2 1.5
CH₂(X³B₁) + CH₃ → CH₂=CH₂ + H						
Methylene + Methyl						
75 LAU/BAS1	EX	295	6.0(13)			2 1.3
75 PIL/ROB Computer fit.	DE	298	3.0(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 OLS/GAR Shock-waves. Absorption-spectroscopy. Best data-fit to a proposed mechanism. Total conc.: $\sim 7.2 \times 10^{17}$ molec.cm ⁻³ .	DE	1800-2700	2.00(13)	0	0	2
CH₂(X³B₁) + CH₄ → CH₃CH₃						
Methylene + Methane						
73 HAL/CRU ¹⁾ k _{ref} : CH ₂ (X ³ B ₁) + CH ₃ CH ₂ CH ₂ CH ₃ → CH ₃ (CH ₂) ₃ CH ₃	RL	304	(4.3±0.2)(-1)			2/2
73 HAL/CRU ¹⁾ k _{ref} : CH ₂ (X ³ B ₁) + CH ₃ CH ₂ CH ₂ CH ₃ → CH ₃ (CH ₂) ₃ CH ₃ (a) → (CH ₃) ₂ CHCH ₂ CH ₃ (b)	RL	304	(2.3±0.1)(-1)			2/2
¹⁾ Limiting high-pressure k.						
CH₂(X³B₁) + CH₂=N=N → CH₂=CH₂ + N₂						
Methylene + Methane, diazo-						
71 BEL Diazomethane/Propane Photolysis. Gas-Chromatography. Estimated ratio. k _{ref} : CH ₂ + CH ₃ CH ₂ CH ₃ → CH ₃ + CH ₃ CH ₂ CH ₂ (a) → CH ₃ + (CH ₃) ₂ CH (b)	RL	298	(4.0±1.0)(2)			2/2
CH₂(a¹A₁) + CH₂=N=N → CH₂=CH₂ + N₂						
Methylene + Methane, diazo-						
71 BEL Diazomethane/Propane Photolysis. Gas-Chromatography.	ES	298	(1.87±0.60)(13)			2
81 HAT/BAN Diazomethane photolysis in air or N ₂ , in presence of H ₂ O. k _{ref} : CH ₂ (¹ A ₁) + H ₂ O → CH ₃ OH. P(Diazomethane) ~ 9 mtorr. P(air, or N ₂) = 760 torr. P(H ₂ O) = (0-4) torr.	RL	298	(1.8±0.6)(1)			2/2
CH₂(X³B₁) + CH≡CH → CH₂=C=CH₂ (a) → CH₃C≡CH (b)						
Methylene + Ethyne						
74 LAU/BAS k _a + k _b . Limiting high-pressure k.	EX	298	(4.52±0.60)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 PIL/ROB $k_a + k_b$.	ES	298	2.41(12)				2
79 VIN/DEB2 $k_a + k_b$. CH=CH oxidation. Fast-flow. The intermediate step: $CH_2(X^3B_1) + CH=CH \rightarrow CH_2C=CH + H$ is suggested, leading to the products of channels (a) and (b). P(Total) = 2.2 torr.	EX	295	(7.83±1.81)(11)				2
$CH_2(X^3B_1) + CH_3CH_3 \rightarrow CH_3CH_2CH_3$							
Methylene + Ethane							
73 HAL/CRU ¹⁾ $k_{ref}: CH_2(X^3B_1) + CH_4 \rightarrow CH_3CH_3$	RL	304	2.52				2/2
73 HAL/CRU ¹⁾	RN	304	2.89(12)				2
73 HAL/CRU ¹⁾ $k_{ref}: CH_2(X^3B_1) + CH_3CH_2CH_2CH_3 \rightarrow CH_3(CH_2)_3CH_3$	RL	304	(1.08±0.01)				2/2
73 HAL/CRU ¹⁾ $k_{ref}: CH_2(X^3B_1) + CH_3CH_2CH_2CH_3 \rightarrow CH_3(CH_2)_3CH_3$ (a) $\rightarrow (CH_3)_2CHCH_2CH_3$ (b)	RL	304	(5.8±0.1)(-1)				2/2
73 HAL/CRU ¹⁾ $k_{ref}: CH_2(X^3B_1) + (CH_3)_3CH \rightarrow (CH_3)_2CHCH_2CH_3$	RL	304	(7.4±0.4)(-1)				2/2
73 HAL/CRU ¹⁾ $k_{ref}: CH_2(X^3B_1) + (CH_3)_3CH \rightarrow (CH_3)_2CHCH_2CH_3$ (a) $\rightarrow (CH_3)_4C$ (b)	RL	304	(6.5±0.3)(-1)				2/2
¹⁾ Insertion at primary CH bond.							
$CH_2(a^1A_1) + CH_2=C=O \rightarrow CH_2=CH_2 + CO$							
Methylene + Ethenone (Ketene)							
74 LAU/BAS M = He. Limiting high-pressure k.	EX	298	(1.93±0.72)(13)				2
77 PIL/ROB	ES	298	2.11(12)				2
$CH_2(a^1B_1) + CH_2=C=O \rightarrow CH_2=CH_2 + CO$							
Methylene + Ethenone (Ketene)							
77 PIL/ROB	ES	298	1.81(13)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CD₂ + CD₂=C=O → CD₂=CD₂ + CO						
Methylene-d ₂ + Ethenone-d ₂ (Ketene-d ₂)						
71 MCN/KEL	RL	653	6.6			2/2
k_{ref} :						
$CD_2 + (CH_3)_4C \rightarrow CD_2H + (CH_3)_3CCH_2$						
CH₂(X³B₁) + CH₃CH₂CH₃ → CH₃CH₂CH₂CH₃ (a)						
→ (CH₃)₃CH (b)						
Methylene + Propane						
73 HAL/CRU	RL	304	3.32			2/2
$(k_a + k_b)/k_{ref}$.						
k_{ref} :						
$CH_2(X^3B_1) + CH_4 \rightarrow CH_3CH_3$						
73 HAL/CRU	RL	304	(8.0±0.2)(-1)			2/2
$(k_a + k_b)/k_{ref}$.						
k_{ref} :						
$CH_2(X^3B_1) + CH_3CH_2CH_2CH_3 \rightarrow CH_3(CH_2)_3CH_3$ (a)						
$\rightarrow (CH_3)_2CHCH_2CH_3$ (b)						
73 HAL/CRU	RN	304	3.79(12)			2
$k_a + k_b$.						
73 HAL/CRU ¹⁾	ES	304	2.65(12)			2
k_a . Insertion at primary CH bond.						
73 HAL/CRU ¹⁾	ES	304	1.14(12)			2
k_b . Insertion at secondary CH bond.						
¹⁾ Recalculated from the reported 1.20 efficiency of CH ₂ insertion at secondary over primary bonds in Propane.						
73 HAL/CRU	RL	304	1.02			2/2
k_a/k_{ref} .						
Insertion at primary CH bond.						
k_{ref} :						
$CH_2(X^3B_1) + CH_3CH_2CH_2CH_3 \rightarrow CH_3(CH_2)_3CH_3$						
73 HAL/CRU	RL	304	(4.4±0.11)(-1)			2/2
k_b/k_{ref} .						
Insertion at secondary CH bond.						
k_{ref} :						
$C_2(X^3B_1) + CH_3CH_2CH_2CH_3 \rightarrow CH_3(CH_2)_3CH_3$						
73 HAL/CRU	RL	304	(2.4±0.11)(-1)			2/2
k_b/k_{ref} .						
Insertion at secondary CH bond.						
k_{ref} :						
$C_2(X^3B_1) + CH_3CH_2CH_2CH_3 \rightarrow CH_3(CH_2)_3CH_3$ (a)						
$\rightarrow (CH_3)_2CHCH_2CH_3$ (b)						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2(a^1A_1) + \text{CH}_3\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_3\text{CH}$ (b)						
Methylene + Propane						
71 BEL ¹) k _a .	ES	298	(2.65±0.72)(12)			2
71 BEL ¹) k _b .	ES	298	(1.14±0.30)(12)			2
71 BEL ¹) k _a + k _b .	ES	298	(3.79±1.02)(12)			2
¹) Dizomethane-Propane Photolysis. Gas-chromatography.						
75 ZAB/CAR k _a + k _b . k _{ref} :	RL	298	1.67(1)			2/2
$\text{CH}_2(a^1A_1) + \text{M} \rightarrow \text{CH}_2(X^3B_1) + \text{M}$.						
$\text{CH}_2(a^1A_1) + \text{CH}_2=\text{CHCH}=\text{CH}_2 \rightarrow \text{cis-CH}_2\text{CH}=\text{CHCH}=\text{CHCH}_3$ (a) $\rightarrow \text{trans-CH}_2=\text{CHCH}=\text{CHCH}_3$ (b) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2$ (c)						
$\rightarrow \triangle_{\text{CH}=\text{CH}_2}$ (d)						
Methylene + 1,3-Butadiene						
75 CRA/ROS (k _a + k _b + k _c)/k _d . Bond insertion versus bond addition.	RL	298	1.4(-1)			2/2
$\text{CH}_2(X^3B_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3$ (b)						
Methylene + Butane						
73 HAL/CRU (k _a + k _b)/k _{ref} . k _{ref} :	RL	304	4.28			2/2
$\text{CH}_2(X^3B_1) + \text{CH}_4 \rightarrow \text{CH}_3\text{CH}_3$						
73 HAL/CRU k _a + k _b .	RN	304	4.88(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
73 HAL/CRU ¹⁾ k _a . Insertion at primary CH bond.	ES	304	2.59(12)			2	
73 HAL/CRU ¹⁾ k _b . Insertion at secondary CH bond.	ES	304	2.29(12)			2	
¹⁾ Recalculated from the reported 1.31 efficiency of CH ₂ insertion at secondary over primary CH bonds in Butane.							
73 HAL/CRU k _b /k _a . Secondary versus primary CH insertion.	RL	304	(8.8±0.1)(-1)			2/2	
$\text{CH}_2(a^1A_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3^\ddagger \text{ (a)}$ $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3^\ddagger \text{ (b)}$							
Methylene + Butane							
72 GRO/HAS ¹⁾ (k _a + k _b)/k _{ref} .	RL	298	1.89			2/2	
72 GRO/HAS ¹⁾ k _b /k _{ref} .	RL	298	(8.9±0.07)(-1)			2/2	
¹⁾ k _{ref} : $\text{CH}_2(a^1A_1) + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3^\ddagger$							
$\text{CH}_2(X^3B_1) + (\text{CH}_3)_3\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_3 \text{ (a)}$ $\rightarrow (\text{CH}_3)_4\text{C} \text{ (b)}$							
Methylene + Propane, 2-methyl-							
73 HAL/CRU (k _a + k _b)/k _{ref} . k _{ref} : CH ₂ (X ³ B ₁) + CH ₄ → CH ₃ CH ₃	RL	304	3.89			2/2	
73 HAL/CRU k _a + k _b .	RN	304	4.46(12)			2	
73 HAL/CRU ¹⁾ k _a . Insertion at primary CH bond.	ES	304	3.88(12)			2	
73 HAL/CRU ¹⁾ k _b . Insertion at tertiary CH bond.	ES	304	5.80(12)			2	
¹⁾ Recalculated from the reported 1.33 efficiency of CH ₂ insertion at secondary over primary CH bonds in 2-Methylpropane.							
73 HAL/CRU k _b /k _a . Tertiary versus primary CH insertion.	RL	304	(1.5±0.1)(-1)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A	k err. units factor
$\text{CH}_2(a^1A_1) + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a)							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ (b)							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (c)							
Methylene + Pentane							
75 ZAB/CAR	RL	298	1.11(1)				2/2
$k_a + k_b + k_c$.							
$k_{\text{ref}}: \text{CH}_2(a^1A_1) + \text{M} \rightarrow \text{CH}(X^3B_1) + \text{M}$.							
$\text{CD}_2 + (\text{CH}_3)_4\text{C} \rightarrow \text{CD}_2\text{H} + (\text{CH}_3)_3\text{CCH}_2$							
Methylene-d ₂ + Propane, 2,2-dimethyl-							
71 MCN/KEL	RL	653	(2.1±0.5)				2/2
$k_{\text{ref}}: \text{CD}_2 + \text{CD}_2=\text{C}=\text{O} \rightarrow \text{CD}_3 + \text{CD}=\text{C}=\text{O}$							
71 MCN/KEL	RN	653	1.5(11)			2	1.5
$\text{CH}_3 (+ \text{M}) \rightarrow \text{CH}_2 + \text{H} (+ \text{M})$							
Methyl							
80 BHA/FRA	EX	1700-2300	6.1(15)	0	44900		2
M = Ar. Shock-tube. Atomic Resonance-Absorption.							
80 ROT/BAR	EX	2150-2850	1.95(16)	0	46100		2
M = Ar. Ethane Thermolysis behind shock-waves.							
Atomic Resonance-Absorption. Same data in 79 ROT/ BAR and 80 ROT. Total conc. $\sim 4.0 \times 10^{18}$ molec.cm ⁻³ .							
$\text{CH}_3 + \text{O}_2 (+ \text{M}) \rightarrow \text{HCHO} + \text{O} + \text{H} (+ \text{M})$ (a)							
$\rightarrow \text{CH}_3\text{O} + \text{O} (+ \text{M})$ (b)							
$\rightarrow \text{CO} + \text{OH} + \text{H}_2 (+ \text{M})$ (c)							
$\rightarrow \text{HCHO} + \text{OH} (+ \text{M})$ (d)							
$\rightarrow \text{CH}_3\text{O}_2 (+ \text{M})$ (e)							
Methyl + Oxygen molecule							
80 BHA/FRA	EX	1700-2300	7.0(12)	0	12910		2
k_a . Shock-tube. Absorption-spectrometry.							
75 BRA/BRO	EX	1200-1800	2.4(13)	0	14500		2
k_b .							
78 REI/ROM	CO	300-2000	1.69(13)	0	15350		2
k_b . RRKM calculation.							
72 SKI/LIF	ES	1000-2500	4.0(12)	0	9059		2
k_c .							
75 BOW1	ES	1900-2400	1.2(11)	0	5000		2
k_d . Best data-fit.							
76 TSU	DE	1500-2000	9.0(11)	0	6014		2
k_d . Computer calculation.							
76 WAS/BAY	EX	259-341	1.74(11)	0	940±250	2	2.24
k_d .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 CLA/IZO2 k _d . Shock-waves and TOF Mass-spectrometry. Total conc. = 9x10 ¹³ molec.cm ⁻³ .	ES	1350	1.99(10)				2
71 DEA/KIS k _d . Shock-waves. Best data-fit. Total conc. = 5x10 ¹⁷ molec.cm ⁻³ .	DE	1750-2575	3.01(13)	0	5033		2
71 IZO/KIS k _d . Shock waves. Best data-fit. Total conc. = 5x10 ¹⁷ molec.cm ⁻³ .	DE	1400-2200	1.20(12)	0	6291		2
78 OLS/GAR k _d . Shock-waves. Absorption-spectroscopy. Best data-fit. Total conc. = ~7.2x10 ¹⁷ molec.cm ⁻³ .	DE	1800-2700	6.92(11)	0	4530		2
78 REI/ROM k _d . RRKM Calculation.	CO	300-2000	1.69(11)	0	4982		2
79 KLA/AND k _d . Flash-photolysis. Resonance-fluorescence. Upper-limit k.	EX	368	≤1.81(8)				2
79 TAB/BAU k _d . M = Ar. CH ₄ oxidation in shock-waves. Best data-fit on the basis of a proposed mechanism. Total conc. = (2.3-4.4)x10 ¹⁸ molec.cm ⁻³ .	ES	1950-2770	2.70(12)	0	6039		2
80 BHA/FRA k _d . Shock-tube. Atomic Resonance-Absorption Spectrometry. Upper-limit k.	EX	1700-2300	≤5.2(13)	0	17400		2
80 BOR/ZAM k _d . Spontaneous ignition of CH ₄ /O ₂ /N ₂ O mixtures.	EX	880-1670	2.00(12)	0	6714		2
80 WAS k _d . M = He. Generation of CH ₃ by reaction of O with CH ₂ =CH ₂ . Fast-flow reactor. Photoionization Mass-spectrometry. k measurements by both, Stern-Volmer plots and steady-state. Comparable data given in 79 WAS1, 79 WAS2, and 79 WAS3. P(CH ₂ =CH ₂) ₀ = (0.30-0.65) mtorr. P(O) ₀ = (0.04-0.19) mtorr. P(Total) = (1.9-6.0) torr. P(O ₂) = (48-229) mtorr.	EX	298	(1.02±0.96)(10)				2
81 BOR/DRA k _d . Combustion of CH ₄ /O ₂ mixtures behind reflected shock-waves. P = 750 torr.	EX	880-1670	2.00(12)	0	6670		2
82 PAR k _d . Reaction of CH ₄ with O ₂ in single-pulse shock-waves. Mass-spectrometry.	EX	1097	3.96(10)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 PLU/RVA2 k _d . Reaction of CH ₃ with O ₂ in a flow-reactor, in He. CH ₃ generated by reacting F with CH ₄ . F atoms generated by dissociation of CF ₄ in a microwave-discharge. Mass-spectrometry. Upper-limit k. [CH ₃] ₀ = (3.7-9.3)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] ₀ = (2.5-7.5)x10 ¹¹ molec.cm ⁻³ . [He] = (0.2-2.1)x10 ¹⁷ molec.cm ⁻³ . [CH ₄] = (8-12)x10 ¹² molec.cm ⁻³ . [O ₂] = 5.2x10 ¹⁵ molec.cm ⁻³ .	EX	295	≤1.81(8)			2
71 VAN/CAL k _e . M = CH ₃ CH ₂ CH ₃ . Limiting high pressure k.	ES	295	~1.1(12)			2
72 BAS/JAM k _e . M = N ₂ , or (CH ₃) ₄ C. Limiting high-pressure k.	EX	295	(3.1±0.3)(11)			2
73 SOK/NIK k _e . M = He. Limiting high-pressure k.	EX	453	1.5(12)			2
75 LAU/BAS2 k _e . M = He, Ar, N ₂ . Limiting high-pressure k.	RN	298	1.02(12)			2
77 HOC/GHO k _e . M = H ₂ . Limiting high-pressure k.	EX	295	(1.3±0.2)(12)			2
77 PAR k _e . M = N ₂ . Limiting high-pressure k.	EX	298	(7.23±3.61)(11)			2
72 BAS/JAM k _e . M = (CH ₃) ₄ C. Low-pressure k.	EX	295	(3.6±0.3)(17)			3
72 BAS/JAM k _e . M = N ₂ . Low-pressure k.	EX	295	(9.4±0.3)(16)			3
73 SOK/NIK k _e . M = He. Low-pressure k.	EX	453	3.9(16)			3
77 PAR k _e . M = N ₂ . Low-pressure k.	EX	298	(1.12±0.79)(17)			3
77 PAR k _e . M = (CH ₃) ₄ C. Low-pressure k.	EX	298	(5.44±2.90)(17)			3
80 WAS k _e . M = He. Generation of CH ₃ by reaction of O with CH ₂ =CH ₂ Fast-flow reactor. Photoionization Mass-spectrometer. k measurements by both, Stern-Volmer plots and steady-state. Comparable data given in 79 WAS1, 79 WAS2 and 79 WAS3. P(Total) = (1.9-6.0) torr. P(CH ₂ =CH ₂) ₀ = (0.30-0.65) mtorr. P(O) ₀ = (0.04-0.19) mtorr. P(O ₂) = (48-339) torr.	EX	298	(5.80±4.35)(16)			3

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 PLU/RYA2 k _e . Flow-reactor. CH ₃ generated by reacting F with CH ₄ in He. F atoms generated by dissociation of CF ₄ in a Microwave-discharge. Limiting low-pressure k. [CH ₃] ₀ = (3.7-9.3)x10 ¹⁰ molec.cm ⁻³ . [CF ₄] ₀ = (2.5-7.5)x10 ¹¹ molec.cm ⁻³ . [He] = (0.2-2.1)x10 ¹⁷ molec.cm ⁻³ . [CH ₄] = (8-12)x10 ¹² molec.cm ⁻³ . [O ₂] = 5.2x10 ¹⁵ molec.cm ⁻³ .	EX	295	(1.23±0.40)(17)			3
CD ₃ + O ₂ → DCDO + OD Methyl-d ₃ + Oxygen molecule						
80 CHI/SKI CD ₄ oxidation in CD ₄ /O ₂ /Ar behind reflected shock-waves. Resonance-absorption spectroscopy.	EX	1700-2200	6.8(11)	0	4571	2
CH ₃ + O ₃ → CH ₃ O + O ₂ (a) → HCHO + H + O ₂ (b)						
Methyl + Ozone						
75 SIM/HEI ¹⁾	RL	221	1.2			2/2
75 SIM/HEI ¹⁾	RL	298	2.2			2/2
¹⁾ (k _a + k _b)/k _{ref} . k _{ref} : CH ₃ + O ₂ → CH ₃ O ₂						
75 SIM/HEI k _a + k _b .	RN	221-298	3.25(12)	0	528	2
80 WAS/AKI M = He. Generation of CH ₃ by reaction of O with CH ₂ =CH ₂ . Fast-flow. Photoionization Mass-Spectrometry. k measurements by Stern-Volmer plots. 3 other possible channels suggested. Comparable data reported in 79 WAS1, 79 WAS2 and 79 WAS3. P(O) ₀ = (0.16-0.40) mtorr. P(CH ₂ =CH ₂) ₀ = (0.36-0.45) mtorr. P(Total) = (1.9-5.7) torr.	EX	298	(4.22±1.63)(11)			2
81 OGR/PAL ²⁾ n = 0 assumed.	EX	243-384	(3.25±0.90)(12)	0	216±80	2
81 OGR/PAL ²⁾ The preexponential factor expressed as: A(T/298) ^{0.71} .	EX	243-384	(1.56±0.42)(12)	0.71	0	2
²⁾ k _a + k _b . M = He. Flash-photolysis of CH ₃ O ₂ at 193 nm. with an ArF laser, in a O ₃ /O ₂ /He mixture. P(Total) = (2-4) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃ + H₂ → CH₄ + H						
Methyl + Hydrogen molecule						
72 SHA/WES k _{ref} : CH ₃ + D ₂ → CH ₃ D + D.	RL	398-718	(9.11±0.20)(-1)	0	-668±12	2/2
73 CLA/DOV2	EX	1340	(4.6±1.4)(10)			2
73 CLA/DOV2	ES	1200-2000	1.55(13)	0	7801	2 2.0
74 KOB/FAC The preexponential factor expressed as: A(T/298) ^{2.0} .	EX	372-1370	7.05(10)	2.0	4811	2
81 MAR/SHA Azomethane Decomposition in H ₂ . Flow-system. P(Total) = (5-26) torr.	EX	584-671	5.01(11)	0	5293	2
CH₃[*] + H₂ → CH₄ + H						
Methyl + Hydrogen molecule						
73 TIN/WES k _{ref} : CH ₃ [*] + CH ₃ Br → CH ₄ + CH ₂ Br. CH ₃ [*] is a 'hot' radical formed by photolysis of CH ₃ Br at 185 nm.	RL	298	(7.5±0.25)(-2)			2/2
CH₃ + HD → CH₄ + D						
Methyl + Deuterium hydride						
72 SHA/WES k _{ref} : CH ₃ + DH → CH ₃ D + H	RL	398-718	(2.83±2.58)(-1)	0	-971±347	2/2
CH₃ + D₂ → CH₃D + D						
Methyl + Deuterium molecule						
76 PRA/ROG2	EX	300-1118	1.60(12)	0	6369±41	2 1.08
77 YAN k _{ref} : CH ₃ + CH ₃ CH=CH ₂ → CH ₄ + CH ₂ CH=CH ₂ Estimated ratio.	RL	1260-1390	3.4(-1)			2/2
CH₃[*] + D₂ → CH₃D + D						
Methyl + Deuterium molecule						
73 TIN/WES k _{ref} : CH ₃ [*] + CH ₃ Br → CH ₄ + CH ₂ Br. CH ₃ [*] is a 'hot' radical formed by photolysis of CH ₃ Br at 185 nm.	RL	298	(8.00±0.13)(-2)			2/2
CD₃ + H₂ → CD₃H + H						
Methyl-d ₃ + Hydrogen molecule						
72 SHA/WES k _{ref} : CD ₃ + D ₂ → CD ₄ + D.	RL	398-718	(1.592±0.124)	0	-296±35	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CD₃[*] + H₂ → CD₃H + H						
Methyl-d ₃ + Hydrogen molecule						
73 TIN/WES	RL	298	(9.25±0.65)(-2)			2/2
k _{ref} : CD ₃ [*] + CD ₃ Br → CD ₄ + CD ₂ Br.						
CD ₃ [*] is a 'hot' radical formed by photolysis of CD ₃ Br at 185 nm.						
CD₃ + HD → CD₃H + D						
Methyl-d ₃ + Deuterium hydride						
72 SHA/WES	RL	398-718	(9.32±1.33)(-1)	0	-275±66	2/2
k _{ref} : CD ₃ + DH → CD ₄ + H.						
CD₃[*] + D₂ → CD₄ + D						
Methyl-d ₃ + Deuterium molecule						
73 TIN/WES	RL	298	(2.15±0.20)			2/2
k _{ref} : CD ₃ [*] + H ₂ → CD ₄ H + H.						
CD ₃ [*] is a 'hot' radical formed by photolysis of CD ₃ Br at 185 nm.						
CH₃ + SO₂ (+ M) → CH₃SO₂ (+ M)						
Methyl + Sulfur dioxide						
74 JAM/KER	EX	298	(1.75±0.25)(11)			2
Azomethane Flash-photolysis. M = Ar, or N ₂ .						
P-independent k. P(Total) = (50-200) torr.						
Same data given in 73 JAM/KER.						
CH₃ + NO (+ M) → CH₃NO (+ M)						
Methyl + Nitrogen oxide (NO)						
71 VAN/CAL	EX	295	(1.00±0.15)(13)			2
M = N ₂ , or Propane. Limiting high-pressure k.						
72 DAV/COR	RL	295	6.2(-1)			2/2
k _{ref} : CH ₃ + NO ₂ → CH ₃ NO ₂						
74 TIT/BAL	EX	443	1.8(12)			2 1.1
M = (CH ₃) ₂ CO. Limiting high-pressure k.						
75 LAU/BAS2	RN	298	1.93(13)			2
M = He, Ar, N ₂ . Limiting high-pressure k. RRKM fit.						
76 FIL/ROB	EX	298	(7.23±0.60)(12)			2
M = Ar, or SF ₆ . RRKM extrapolation of data.						
Limiting high-pressure k.						
74 PRA/VEL	EX	295	(1.0±0.1)(17)			3
M = He.						
74 TIT/BAL	EX	443	6.1(18)			3
M = (CH ₃) ₂ CO. Low-pressure k.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 FRA/VEL2 M = He. RRKM calculation.	CO	325-521	7.24(16)	0	-211±10	3	1.20
80 WAS CH ₃ generated by reacting O with Ethene. Fast-flow. Photoionization Mass-spectrometry. Comparable data in 79 WAS1, 79 WAS2 and 79 WAS3. P(He) = (1.8-6.3) torr. P(CH ₂ =CH ₂) ₀ = (0.45-0.57)mtorr. P(O) ₀ = (0.15-0.31) mtorr.	EX	298	(8.71±2.90)(17)			3	
$\text{CH}_3 + \text{NO}_2 (+ \text{M}) \rightarrow \text{CH}_3\text{O} + \text{NO} (+ \text{M})$ (a) $\rightarrow \text{CH}_3\text{ONO} (+ \text{M})$ (b) $\rightarrow \text{CH}_3\text{NO}_2 (+ \text{M})$ (c)							
Methyl + Nitrogen oxide (NO ₂)							
74 GLA/TRO2 -k _a .	EX	1100-1400	1.3(13)	0	0	2	
81 YAM/SLA k _a . CH ₃ produced by IR Multiphoton dissociation of C ₆ F ₅ OCH ₃ in He. Photoionization Mass-spectrometry. [NO ₂] = (1.10-3.31)x10 ¹² molec.cm ⁻³ . [CH ₃] ₀ = 1.1x10 ¹¹ molec.cm ⁻³ . P(Total) = 1 torr.	EX	295	(1.51±0.30)(13)			2	
72 DAV/COR k _b /k _c .	RL	295	2.17			2/2	
74 GLA/TRO2 ¹⁾ k _c . M = Ar. Estimated, limiting high-pressure k.	RN	300-1400	≈2.07(13)	-0.6	0	2	
74 GLA/TRO2 ¹⁾ k _c . M = Ar. Estimated, low-pressure k. Rate constant expressed as k/[Ar].	RN	300-1400	≈3.58(20)	-6.0	0	3	
¹⁾ Preexponential factor expressed as: A(T/298) ⁿ .							
$\text{CH}_3 + \text{N}_2\text{O} \rightarrow \text{CH}_3\text{O} + \text{N}_2$							
Methyl + Nitrogen oxide (N ₂ O)							
73 FAL/HOA	RN	873	(1.4±0.3)(7)			2	
77 BOR/ZAM Estimated, upper-limit k.	ES	1000-2000	<1.0(15)	0	14276	2	
$\text{CH}_3 + \text{CO} (+ \text{M}) \rightarrow \text{CH}_3\text{CO} (+ \text{M})$ (a) $\rightarrow \text{CH}=\text{CH} + \text{OH} (+ \text{M})$ (b)							
Methyl + Carbon monoxide							
74 WAT/WOR k _a .	RN	260-296	1.58(11)	0	3007±12	2	1.58
82 ANA/MAW ¹⁾ k _a . Limiting high-pressure k.	EX	303	9.64(6)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ANA/MAW ¹) k _a . Limiting high-pressure k.	EX	343	3.43(7)			2
81 PAR ²) k _a . P(CO) = 100 torr.	EX	298	(1.08±0.12)(6)			3
81 PAR ²) k _a . P(CO) = 750 torr.	EX	298	(3.61±0.60)(6)			3
82 ANA/MAW ¹) k _a . Limiting low-pressure k.	EX	303	2.07(12)			3
82 ANA/MAW ¹) k _a . Limiting low-pressure k.	EX	343	3.88(12)			3
81 TSU/KAT k _p . M = Ar. Thermal oxidation of CH ₃ OH/O ₂ behind reflected shock-waves. UV-absorption. IR-emission. Same data given in 81 TSU/HAS. ¹) M = CO. Molecular modulation. CH ₃ produced by photolysis of Azoethane. [Azomethane] = 1.0x10 ¹⁷ molec.cm ⁻³ . [CO] = (0.3-2.7)x10 ¹⁹ molec.cm ⁻³ . ²) Photolysis of Acetone at (25.4-40.0) nm. Molecular modulation.	ES	1500-1900	3.80(13)	0	30432	2
CH ₃ + CH ₃ (+ M) → CH ₃ CH ₂ + H (+ M) (a) → CH ₂ =CH ₂ + H ₂ (+ M) (b) → CH ₃ CH ₃ (+ M) (c)						
Methyl						
80 ROT/BAR k _a . CH ₃ CH ₃ thermolysis behind shock-waves. Atomic Resonance-Absorption. Computer simulation. Decomposition of CH ₃ CH ₂ to CH ₂ =CH ₂ + H is suggested. Total conc. ~ 4.0x10 ¹⁸ molec.cm ⁻³ . Same data given in 79 ROT/JUS2 and 80 ROT.	DE	2150-1850	8.01(14)	0	13400	2
81 CHI/SKI2 k _a . M = Ar. Ethane pyrolysis behind reflected shock-waves. Resonance-absorption spectroscopy. Decomposition of CH ₃ CH ₂ is suggested. Data-fit. P(Total) = (2-3) atm.	ES	1240-1700	4.0(14)	0	13387	2
78 TSU k _a + k _b . Shock-tube.	EX	1396-2396	9.7(15)	0	15396	2
75 GAR/OWE k _b .	EX	2000-2651	6.0(16)	0	21651	2
71 CLA/IZO1 k _c . Shock-waves. TOF Mass-spectrometry.	EX	1120-1400	(8.4±3.6)(12)	0	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 TEN/JON k _c . Data-fit to a proposed mechanism.	CO	303-603	2.63(13)	0	216	2
73 BAS/LAU k _c . M = He. Limiting high-pressure k.	EX	298	(5.74±0.71)(13)			2
73 BAY/BRO k _c .	EX	295	(2.4±0.2)(13)			2
73 TRU/RIC k _c . M = N ₂ . Limiting high-pressure k.	EX	313	(2.41±0.18)(13)			2
74 JAM/SIM k _c . M = Ar. Limiting high-pressure k.	EX	298	(3.37±0.46)(13)			2
74 POH/LEI k _c . M = He, or N ₂ , or N ₂ + CO.	EX	298	(2.7±0.3)(13)			2
76 CAL/MET k _c .	EX	295	(3.31±0.18)(13)			2
76 GLA/QUA k _c . M = Ar. Limiting high-pressure k. Average k at highest concentrations.	EX	1200-1500	(1.02±0.36)(13)			2
76 PAR/PAU k _c . M = N ₂ .	EX	250-450	(2.41±0.52)(13)			2
76 VAN k _c . Extrapolated, limiting high-pressure k.	EX	1350	2.0(13)			2 1.5
77 GLA/QUA k _c . M = Ar. Limiting high-pressure k.	EX	1400	(1.75±0.90)(13)			2
77 HEL/MAN k _c . Flow-reactor. UV absorption spectroscopy. Limiting high-pressure k. P = (10-80) torr.	ES	1005	1.41(13)			2
77 HOC/GHO k _c . M = N ₂ . Limiting high-pressure k.	EX	295	(3.1±0.6)(13)			2
78 PAC/WIM k _c . Neopentane flow-pyrolysis. P = 7.6 torr.	CO	821	2.1(13)			2
79 SEP/MAR ¹⁾ P(Ar) ~ 14 torr.	EX	750	5.0(12)			2
79 SEP/MAR ¹⁾ P(Ar) = 7.4 torr.	EX	640-818	3.98(12)			2
¹⁾ k _c . Discharge-flow. Best-fit.						
79 ZAS/SMI k _c . M = Ar. Tetramethyltin decomposition behind incident and reflected shock-waves. High-pressure k. [Ar] = (0.1-5.5) × 10 ¹⁹ molec.cm ⁻³ .	EX	1750	(1.33±0.66)(13)			2
80 ADA/BAS2 k _c . Azomethane Flash-photolysis. Absorption spectroscopy.	EX	298	(3.2±0.4)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 BAU/DUX k _c . Recommended high-pressure k. Critical review.	RE	250-420	2.40(13)	0	0	2	1.2
80 PAC/WIM1 k _c . C(CH ₃) ₄ pyrolysis in a flow-reactor. Extrapolated limiting high-pressure k. P = (4-335) torr.	EX	823	(2.2±0.5)(13)			2	
76 VAN ²⁾ k _c . M = He. Extrapolated limiting low-pressure k.	EX	450	2.3(21)			3	4.0
76 VAN ²⁾ k _c . M = He. Calculated limiting low-pressure k.	CO	450	7.4(21)			3	
76 VAN ²⁾ k _c . M = Ar. Extrapolated limiting low-pressure k.	EX	1350	1.2(19)			3	4.0
76 VAN ²⁾ k _c . M = Ar. Calculated limiting low-pressure k.	CO	1350	2.8(19)			3	2.0
²⁾ Rate constants expressed as k/[M].							
CH₃[*] + CH₃ → CH₄ + CH₂							
Methyl							
77 RIC/TRU Upper-limit k. M = Ar. CH ₃ [*] is an energy-rich radical formed by photolysis of CH ₃ I at 260 nm.	EX	298	≤1.02(14)			2	
CD₃ + CD₃ (+ M) → CD₂=CD₂ + D + D (+ M) (a) → CD₃CD₃ (+ M) (b)							
Methyl-d ₃							
81 CHI/SKI2 k _a . M = Ar. Ethane pyrolysis behind reflected shock-waves. Resonance-absorption. Data-fit to a proposed mechanism. P(Total) = (2-3) atm.	ES	1240-1700	4.0(14)	0	13387	2	
76 CAL/MET k _b . M = N ₂ .	EX	295	(2.95±0.24)(13)			2	
76 GLA/QUA k _b . M = Ar. Limiting high-pressure k. Average k at highest concentrations.	EX	1200-1500	(1.33±0.54)(13)			2	
76 PAR/PAU k _b . M = N ₂ .	EX	298	(2.41±0.52)(13)			2	
77 GLA/QUA k _b . M = Ar. Limiting high-pressure k.	EX	1400	(1.93±1.02)(13)			2	
76 VAN k _b . M = Ar. Extrapolated limiting low-pressure k.	EX	1350	7.0(19)			3	4.0
76 VAN k _b . M = Ar. Calculated limiting low-pressure k.	CO	1350	7.7(19)			3	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃ + CH₄ → CH₃CH₃ + H (a)						
→ CH₃CH₂ + H₂ (b)						
Methyl + Methane						
79 TAB/BAU ¹⁾	ES	1950-2770	8.0(13)	0	20131	2
<i>k_a</i> .						
79 TAB/BAU ¹⁾	ES	1950-2770	1.0(13)	0	11576	2
<i>k_b</i> .						
¹⁾ M = Ar. Methane pyrolysis in shock-waves. Best data-fit on the basis of a proposed mechanism. Total conc.: (1.4-5.4) × 10 ¹⁸ molec.cm ⁻³ .						
CH₃ + CHO → CH₄ + CO (a)						
→ CH₃CHO (b)						
Methyl + Methyl, oxo-						
77 HEL/MAN	ES	1005	3.78(13)			2
<i>k_a</i> . Pyrolysis in a flow-reactor. Absorption-spectroscopy. Gas-chromatography. P = (10-80) torr.						
79 NAD/SAR4	EX	298	>3.01(13)			2
<i>k_a</i> . Intracavity laser spectroscopy. Lower-limit k.						
80 MUL	EX	298	(2.66 ± 0.97)(13)			2
<i>k_b</i> . CH ₃ CHO decomposition by pulsed UV-Photolysis. Internal-resonator Laser-Spectroscopy.						
79 NAD/SAR2	EX	298	(1.39 ± 0.60)(14)			2
<i>k_{overall}</i> . Pulse-photolysis of CH ₃ CHO.						
CH₃ + HCHO → CH₄ + CHO						
Methyl + Formaldehyde						
77 HEL/MAN	ES	1005	3.16(10)			2
Pyrolysis in a flow-reactor. UV-Absorption-spectroscopy. Gas-chromatography. P = (10-80) torr.						
CH₃ + CH₃O → CH₄ + HCHO (a)						
→ CH₃OCH₃ (b)						
Methyl + Methoxy						
79 HAS/KOS ¹⁾	RN	298	2.71(13)			2
<i>k_a</i> .						
79 HAS/KOS ¹⁾	RN	298	3.31(13)			2
<i>k_b</i> .						
¹⁾ Flash-photolysis of CH ₃ COOCH ₃ . k's determined relative to the reaction: CH ₃ + CH ₃ → CH ₃ CH ₃ . P = (1.5-700) torr. Gas-chromatography.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{O} + \text{CH}_3\text{O}$ Methyl + Methylidioxy						
77 PAR	EX	298	(3.61±0.60)(13)			2
$\text{CD}_3 + \text{COS} \rightarrow \text{CD}_3\text{S} + \text{CO}$ Methyl-d ₃ + Carbon oxide sulfide						
72 JAK/AHM	RN	354-490	3.80(11)	0	5712±176	2 1.78
$\text{CH}_3 + \text{CH}_3\text{N}=\text{NH} \rightarrow \text{CH}_4 + \text{CH}_3\text{N}=\text{N}$ Methyl + Diazene, methyl-						
76 VID/WIL	EX	294	(1.31±0.17)(10)			2
$\text{CH}_3 + \text{CH}_3\text{NO}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{NO}_2$ Methyl + Methane, nitro-						
80 BAL/FED Continuous-circulation Molybdenum glass-reactors. Gas-chromatography. P(Total) = (126-133) torr.	EX	413-482	7.07(11)	0	5606±282	2 1.95
$\text{CH}_3 + \text{CH}=\text{CH} \rightarrow \text{CH}_3\text{CH}=\text{CH}$ Methyl + Ethyne						
77 HOL/KER	RN	379-487	6.19(11)	0	3875±755	2 6.31
$\text{CH}_3 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_2=\text{CH}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2$ (b) Methyl + Ethene						
76 CHE/BAC k_a .	RN	1038	1.0(9)			2
79 TAB/BAU k_a . M = Ar. CH_4 pyrolysis in shock-waves. Best data-fit. Total conc.: $(1.4-5.4) \times 10^{18}$ molec. cm^{-3} .	EX	1950-2770	5.0(12)	0	6543	2
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CH}_2=\text{CHF} \rightarrow \text{CH}_3\text{CH}_2\text{CHF}$	RL	335-424	7.24(2)	0	-468±101	2/2 1.07
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CH}_2=\text{CF}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CF}_2$	RL	335-424	4.90(1)	0	-2416±503	2/2 1.23
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CF}_2=\text{CF}_2 \rightarrow \text{CH}_3\text{CF}_2\text{CF}_2$	RL	335-424	8.32(3)	0	1319±554	2/2 1.23
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CH}_2=\text{CHCl} \rightarrow \text{CH}_3\text{CH}_2\text{CHCl}$	RL	335-424	2.88(2)	0	-941±252	2/2 1.10
72 TED/WAL ¹⁾ k_{ref} : $\text{CH}_3 + \text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CHCH}_3$ ¹⁾ k_b/k_{ref} .	RL	335-424	1.07(4)	0	-377±201	2/2 1.07

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 CAM/MAR k _b . Determined from k _{-b} and thermochemical data.	DE	676-813	3.16(10)	0	3969	2	
77 HOL/KER k _b .	RN	350-503	2.09(11)	0	3674±503	2	3.16
CH₃ + CH₃CH₂ → CH₃CH₂CH₃							
Methyl + Ethyl							
72 TEN/JON	CO	303-603	2.51(13)	0	201	2	
75 LIF/FRE1 k ₁ = k ₋₁ K.	DE	1050-1250	2.4(12)			2	
80 KOI/GAR Propane Thermolysis behind reflected shock-waves. Absorption Spectroscopy. Data-fit to a proposed mechanism.	ES	1300-1700	7.24(12)	0	0	2	
82 SIM/GAR ¹⁾ 4.3% Propane in Ar. Conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	ES	1300-1700	8.0(10)	0	-5700	2	
82 SIM/GAR ¹⁾ 5% Propane in Ar. Conc. = 9.0x10 ¹⁸ molec.cm ⁻³ .	ES	1300-1700	9.0(7)	0	-14700	2	
¹⁾ Pyrolysis of Propane in Ar behind reflected shock-waves. Data-fit to a proposed mechanism.							
CH₃ + CH₃CH₃ → CH₄ + CH₃CH₂							
Methyl + Ethane							
71 CLA/IZO1 Shock-waves. Time-of-flight Mass-spectrometry.	ES	1485	3.55(11)			2	
72 PAC/PUR2	EX	920-1040	5.01(14)	0	10826±2406	2	10.
73 CLA/DOV1 BEBO calculation. The preexponential factor expressed as: A(T/298) ^{4.0} .	CO	300-1800	4.34(9)	4.0	4167±15	2	1.02
74 YAM/RYP	RN	980-1130	3.02(12)	0	6844±1107	2	3.16
76 BRA/WES2 Computer simulation optimization.	DE	1055-1325	3.24(13)	0	9057	2	1.78
76 CHE/BAC k for α ~ 1. Measured k values also given at T = 880, 995 and 1068 K. Non-Arrhenius behaviour.	EX	1038	(1.3±0.3)(10)			2	
77 HEL/MAN Flow-reactor pyrolysis. Absorption spectroscopy. Gas-chromatography. P ≈ (10-80) torr.	ES	1005	3.98(9)			2	
79 ROT/JUS2 Shoch-tube. Atomic Resonance-absorption Spectrophotometry. k determined by computer simulation. Total conc. = (0.2-2.3)x10 ¹⁹ molec.cm ⁻³ .	DE	1450-1600	5.00(13)	0	9800	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3\text{CO} \rightarrow \text{CH}_4 + \text{CH}_2=\text{C}=\text{O}$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{CO}$ (b) $\rightarrow (\text{CH}_3)_2\text{CO}$ (c)						
Methyl + Ethyl, 1-oxo- (Acetyl)						
78 ADA/BAS $k_a + k_b + k_c$. Acetone Flash-photolysis Kinetic Spectroscopy. P(Total) = 50 torr.	ES	298	7.5(13)			2
81 ADA/BAS2 $k_a + k_b + k_c$. Acetone Flash-photolysis. Kinetic Spectroscopy.	ES	298	8.6(13)			2
81 ADA/BAS2 $k_b/(k_a + k_b + k_c)$. Acetone Flash-photolysis. Kinetic-Spectroscopy. Estimated ratio.	RL	298	3.8(-1)			2/2
79 HAS/KOS k_c . Flash-photolysis of $\text{CH}_3\text{COOCH}_3$. k determined relative to the reaction: $\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3$. Gas-chromatography. P = (1.5-700) torr.	RN	298	3.30(13)			2
82 ANA/MAW k_c . Average of 24 k values obtained through data-fit. Molecular Modulation Spectroscopy. CH_3 and CH_3CO produced by photolysis of Azomethane in presence of CO. Gas-chromatography. P-inde- pendent k. [Azomethane] = 1.0×10^{17} molec.cm ⁻³ . [CO] = $(0.3-2.7) \times 10^{19}$ molec.cm ⁻³ .	RN	263-343	$(2.26 \pm 0.27)(13)$	0	0	2
82 TIM/KAL k_c . Flash-photolysis of 2,3-Butanedione. Gas-chromatography. $[\text{CH}_3] = (0.26-6.08) \times 10^{18}$ molec.cm ⁻³ . $[\text{CH}_3\text{CO}] = (1.14-5.77) \times 10^{18}$ molec.cm ⁻³ . P = (11-47) torr.	EX	298	$(2.98 \pm 0.17)(13)$			2
$\text{CD}_3 + \text{CD}_3\text{CO} \rightarrow \text{CD}_4 + \text{CD}_2=\text{C}=\text{O}$ (a) $\rightarrow \text{CD}_3\text{CD}_3 + \text{CO}$ (b) $\rightarrow (\text{CD}_3)_2\text{CO}$ (c)						
Methyl-d ₃ + Ethyl-2,2,2-d ₃ -1-oxo- (Acetyl-d ₃)						
81 ADA/BAS2 $k_a + k_b + k_c$. Acetone-d ₆ Flash-photolysis. Kinetic Spectroscopy.	ES	298	5.2(13)			2
81 ADA/BAS2 $k_b/(k_a + k_b + k_c)$. Acetone-d ₆ Flash-photolysis. Kinetic-Spectroscopy. Estimated ratio.	RL	298	4.7(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k/ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CO}$ (a)							
$\rightarrow \text{CH}_4 + \text{CH}_2\text{CHO}$ (b)							
$\rightarrow (\text{CH}_3)_2\text{CHO}$ (c)							
Methyl + Acetaldehyde							
71 BAL/LAN	ES	713-813	(1.6±0.6)(12)	0	4127±252	2	
k_a .							
75 COL/NAE	ES	800-1225	4.37(15)	0	14570	2	
k_b .							
76 BAR/BER	RL	785	2.7			2/2	
$(k_a + k_b)/k_{\text{ref}}$.							
$k_{\text{ref}}: \text{CH}_3 + \text{CH}_3\text{CDO} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CO}$							
75 BAT/MCC	ES	393-473	7.94(10)	0	0±503	2	
k_c .							
$\text{CH}_3 + \text{CH}_3\text{CDO} \rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CO}$ (a)							
$\rightarrow \text{CH}_4 + \text{CH}_2\text{CDO}$ (b)							
Methyl + Acetaldehyde-1-d							
76 BAR/BER	RL	785	6.2(-1)			2/2	
k_b/k_a .							
$\text{CH}_3 + \text{HC(O)OCH}_3 \rightarrow \text{CH}_4 + \text{C(O)OCH}_3$ (a)							
$\rightarrow \text{CH}_4 + \text{HC(O)OCH}_2$ (b)							
Methyl + Formic acid methyl ester (Methyl formate)							
71 DON/DOR ¹⁾	EX	400-513	5.01(11)	0	5184±101	2	1.26
71 DON/DOR ¹⁾	EX	455	5.62(6)			2	
¹⁾ $k_a + k_b$. Acetone photolysis. Mass-spectrometry.							
$\text{CD}_3 + \text{HC(O)OCH}_3 \rightarrow \text{CD}_3\text{H} + \text{C(O)OCH}_3$ (a)							
$\rightarrow \text{CD}_3\text{H} + \text{HC(O)OCH}_2$ (b)							
Methyl-d ₃ + Formic acid methyl ester (Methyl formate)							
71 DON/DOR ¹⁾	EX	400-513	3.55(11)	0	5033±252	2	1.74
71 DON/DOR ¹⁾	EX	455	5.25(6)			2	
¹⁾ k_a . Acetone photolysis. Mass-spectrometry.							
71 DON/DOR ²⁾	EX	400-513	4.37(11)	0	5083±151	2	1.38
71 DON/DOR ²⁾	EX	455	6.17(6)			2	
¹⁾ $k_a + k_b$. Acetone photolysis. Mass-spectrometry.							
$\text{CD}_3 + \text{DC(O)OCH}_3 \rightarrow \text{CD}_4 + \text{C(O)OCH}_3$ (a)							
$\rightarrow \text{CD}_3\text{H} + \text{DC(O)OCH}_2$ (b)							
Methyl-d ₃ + Formic-d acid methyl ester (Methyl formate-d)							
71 DON/DOR ¹⁾	EX	400-513	3.02(11)	0	5888±151	2	1.45
71 DON/DOR ¹⁾	EX	455	6.92(5)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
¹) k_a . Acetone photolysis. Mass-spectrometry.							
71 DON/DOR ²)	EX	400-513	1.23(11)	0	5435±101	2	1.29
71 DON/DOR ²)	EX	455	7.59(5)			2	
²) k_b . Acetone photolysis. Mass-spectrometry.							
¹) Photolysis of Acetone. Mass-spectrometry.							
$\text{CH}_3 + (\text{CH}_3)_2\text{O} \rightarrow \text{CH}_4 + \text{CH}_2\text{OCH}_3$ Methyl + Methane, oxybis- (Dimethyl ether)							
75 PAC	EX	782-936	3.16(13)	0	7578±842	2	2.51
Curved Arrhenius plot over the extended T-range (373-936) K.							
77 HEL/MAN	ES	1005	1.31(10)			2	1.58
Pyrolysis in a flow-reactor. UV-Absorption spectroscopy. Gas-chromatography. P = (10-80) torr.							
82 BAT/ALV ¹)	EX	373-473	2.00(11)	0	4781±101	2	1.26
82 BAT/ALV ¹)	SE	373-935	3.55(12)	0	5939±101	2	1.26
Extended T-range by combining the above k with data found in the literature.							
¹) Photolysis of Azomethane in the presence of Dimethyl ether. P(CH ₃ OCH ₃) = (0-470) torr. P(Azomethane) = 23 torr.							
$\text{CH}_3 + \text{S} \rightarrow \text{CH}_3\text{S} + \text{CH}_2=\text{CH}_2$							
Methyl + Thirane (Ethylene episulfide)							
72 JAK/AHM	RN	304-478	7.08(10)	0	3372±403	2	3.02
$\text{CD}_3 + \text{S} \rightarrow \text{CD}_3\text{H} + \text{S}_2$ (a)							
$\rightarrow \text{CD}_3\text{S} + \text{CH}_2=\text{CH}_2$ (b)							
Methyl-d ₃ + Thirane (Ethylene episulfide)							
72 JAK/AHM	RN	303-477	2.19(11)	0	4801±503	2	3.98
k_a .							
72 JAK/AHM	RN	303-477	5.89(10)	0	3271±554	2	4.37
k_b .							
$\text{CH}_3 + (\text{CH}_3)_2\text{S} \rightarrow \text{CH}_4 + \text{CH}_3\text{SCH}_2$							
Methyl + Methane, thiobis- (Dimethyl sulfide)							
76 ART/LEE	RN	393-518	4.17(11)	0	4613±82	2	1.20

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃ + CH₃N=NCH₃ → CH₄ + CH₃N=NCH₂							
Methyl + Diazene, dimethyl- (Azomethane)							
77 SCH/KNO	RL	524-565	1.0	0	-604±302	2/2	2.0
k _{ref} : CH ₃ + CD ₃ COC OCD ₃ → CH ₃ D + CD ₃ COC OCD ₃							
80 DUR/MAR	EX	323-453	1.07(12)	0	4906±132	2	1.41
Photolysis of 14% Azomethane in Propane at 366 nm. P = (25-300) torr.							
CD₃ + CH₃N=NCH₃ → CD₃H + CH₂N=NCH₃							
Methyl-d ₃ + Diazene, dimethyl- (Azomethane)							
77 SCH/KNO	RL	524-565	6.3(-1)	0	-755±302	2/2	2.0
k _{ref} : CD ₃ + CD ₃ COC OCD ₃ → CD ₄ + CD ₂ COC OCD ₃							
CH₃ + CH₂=C=CH₂ → CH₂C(CH₃)=CH₂							
Methyl + 1,2-Propadiene (Allene)							
73 TSA2	ES	996-1180	1.58(11)	0	2500	2	
1100 K given by the author as central T.							
CH₃ + (CH₃)₂CH → CH₄ + CH₃CH=CH₂ (a)							
→ (CH ₃) ₃ CH (b)							
Methyl + Ethyl, 1-methyl- (Isopropyl)							
72 ARI/STE	RL	295	(2.4±0.3)(-1)			2/2	
k _a /k _b . Azoisopropane photolysis.							
CH₃ + CH₃CH₂CH₃ → CH₄ + CH₃CH₂CH₂ (a)							
→ CH ₄ + (CH ₃) ₂ CH (b)							
Methyl + Propane							
75 CAM/MAR	EX	676-743	2.00(12)	0	5689±818	2	3.31
k _a + k _b . Low-T region.							
75 CAM/MAR	EX	743-813	5.01(15)	0	11595±902	2	3.24
k _a + k _b . High-T region.							
75 LIF/FRE1	EX	1050-1250	3.55(12)	0	5184	2	
k _a + k _b . Data-fit to a proposed mechanism.							
79 PRA/ROGZ	ES	1008	(4.2±1.1)(9)			2	
k _a + k _b . M = Ar. Propane pyrolysis in a wall-less reactor. Average k at the mean experimental T. Other k values within the 967-1051 K T-range are also given. Approximate fit. P(Ar) = 600 torr.							
80 DUR/MAR	RN	323-453	2.6(11)	0	4896±132	2	1.41
k _a + k _b . Photolysis of 14% Azomethane in Propane at 366 nm. P = (25-300) torr. k determined relative to the reaction: CH ₃ + CH ₃ → CH ₃ CH ₃							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref))	n	B, B-B(ref)	k, A units	k err. factor
81 HAU/SAN $k_a + k_b$. Pyrolysis in a flow-reactor. The preexponential factor expressed as: $A(T/298)^n$.	EX	1110-1235	6.23(9)	4.0	4177	2	
$CH_3 + CH_3C(O)CHO \rightarrow CH_4 + CH_3CO + CO$ Methyl + Propanal, 2-oxo-							
77 KYL/ORC	RN	353-444	1.38(11)	0	3332±337	2	2.40
$CH_3 + (CH_3)_2CO \rightarrow CH_4 + CH_2C(O)CH_3$ (a) $\rightarrow (CH_3)_3CO$ (b) $\rightarrow CH_3CH_2CH(CH_3)O$ (c) Methyl + 2-Propanone							
72 SHA/WES k_a/k_{ref} . k_{ref} : $CH_3 + D_2 \rightarrow CH_3D + D$.	RL	398-718	(6.17±0.46)(-1)	0	-1021±38	2/2	
72 SHA/WES k_a/k_{ref} . k_{ref} : $CH_3 + DH \rightarrow CH_3D + H$.	RL	398-718	(2.3±0.92)	0	-413±186	2/2	
76 ART/LEE k_a .	RN	393-518	4.07(11)	0	4869±55	2	1.12
79 ART/NEW1 k_a . Acetone photolysis.	EX	117-244	3.39(11)	0	4882±20	2	1.05
71 CAD/TRO k_b . $k_b = k_{-b}K$.	DE	373-423	1.74(9)	0	6772±902	2	10.0
80 KNO/RIC k_b . Thermolysis of Azomethane and di-t-Butyl peroxide. Mass-spectrometry. k determined relative to reaction: $CH_3 + (CD_3)_2CO \rightarrow CH_3D + CD_2C(O)CD_3$	RN	413-563	3.16(10)	0	5788±554	2	2.51
75 BAT/MCC k_c .	ES	393-473	2.0(11)	0	0±503	2	
$CH_3 + (CD_3)_2CO \rightarrow CH_3D + CD_2C(O)CD_3$ (a) $\rightarrow (CD_3)_2C(CH_3)O$ (b) Methyl + 2-Propanone-1,1,1,3,3,3-d ₆							
80 KNO/RIC ¹⁾ k_a/k_b .	RL	413-563	1.48(1)	0	-151±86	2/2	1.17
80 KNO/RIC ¹⁾ k_b .	RN	413-563	3.16(10)	0	5888±252	2	1.59
¹⁾ Thermolysis of Azomethane and di-t-Butyl peroxide.							
$CD_3 + (CD_3)_2CO \rightarrow CD_4 + CD_3C(O)CD_2$ Methyl-d ₃ + 2-Propanone-1,1,1,3,3,3-d ₆							
72 SHA/WES k_{ref} : $CD_3 + H_2 \rightarrow CD_3H + H$	RL	398-718	(8.56±0.68)(-1)	0	532±36	2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 SHA/WES $k_{ref}: CD_3 + HD \rightarrow CD_3H + D$	RL	398-718	(1.47±0.13)	0	340±42	2/2	
$CH_3 + CH_3C(O)OCH_3 \rightarrow CH_4 + CH_2C(O)OCH_3$ (a) $\rightarrow CH_4 + CH_3C(O)OCH_2$ (b) Methyl + Acetic acid methyl ester (Methyl acetate)							
79 ART/NEW2 ¹⁾ k_a	EX	389-497	1.48(11)	0	5160±212	2	1.66
79 ART/NEW2 ¹⁾ k_b	EX	389-497	2.75(11)	0	5651±155	2	1.45
79 ART/NEW2 ¹⁾ $k_a + k_b$	EX	389-497	3.63(11)	0	5344±117	2	1.32
¹⁾ Photolysis in silica vessel.							
$CH_3 + CH_3C(O)OCD_3 \rightarrow CH_4 + CH_2C(O)OCD_3$ (a) $\rightarrow CH_3D + CH_3C(O)OCD_2$ (b) Methyl + Methan-d ₃ -ol acetate (Methyl-d ₃ acetate)							
81 ART/NEW ¹⁾ k_a	EX	386-505	2.04(11)	0	5232±124	2	1.32
81 ART/NEW ¹⁾ k_b	EX	386-505	2.14(11)	0	6430±77	2	1.20
¹⁾ Photolysis in silica vessel.							
$CH_3 + CD_3C(O)OCH_3 \rightarrow CH_3D + CD_2C(O)OCH_3$ (a) $\rightarrow CH_4 + CD_3C(O)OCH_2$ (b) Methyl + Acetic acid-d ₃ methyl ester (Methyl acetate-d ₃)							
79 ART/NEW2 k_a	EX	389-497	2.45(11)	0	6268±40	2	1.10
Photolysis in silica vessel.							
$CH_3 + \begin{matrix} S \\ / \backslash \\ H_3C \end{matrix} \rightarrow CH_3S + CH_3CH=CH_2$ (a) $\rightarrow CH_4 + [C_3H_5S]$ (b) Methyl + Thiirane, methyl-							
72 JAK/AHM k_a	RN	339-435	2.14(11)	0	3749±835	2	8.32
72 JAK/AHM k_b	RN	339-435	1.0(11)	0	4157±438	2	3.02

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3 + (\text{CH}_3)_2\text{CHNO}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{CH}(\text{CH}_3)\text{NO}_2$ (a) $\rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CNO}_2$ (b)							
Methyl + Propane, 2-nitro-							
77 BAL/TIT ¹⁾	EX	413-479	1.38(11)	0	4222±257	2	1.74
78 TIT/BAL ¹⁾	EX	413-479	1.26(11)	0	4227±252	2	2.0
¹⁾ $k_a + k_b$. Flow-reactor. P(Total) 100 torr.							
$\text{CH}_3 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$							
Methyl + 2-Propenyl, 2-methyl-							
73 TSA2 1020 K given by the author as central-T.	EX	996-1180	2.0(13)			2	
$\text{CH}_3 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{CH}=\text{CHCH}_3$							
Methyl + 2-Butene, (Z)-							
73 RIC/MAR k_{ref} : $\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CO}$	RL	768	≈8.0			2/2	
$\text{CH}_3 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$							
Methyl + 1-Propene, 2-methyl-							
73 KON/MAR	ES	770-855	1.12(14)	0	8858	2	
73 RIC/MAR k_{ref} : $\text{CH}_3 + \text{CH}_3\text{CHO} \rightarrow \text{CH}_4 + \text{CH}_3\text{CO}$	RL	768	≈5.0			2/2	
76 BRA/WES1 ¹⁾	EX	1030-1300	2.6(16)	0	13352	2	6.61
76 BRA/WES2 ¹⁾	DE	1055-1325	6.8(13)	0	9803	2	1.62
¹⁾ Computer data-fit to a proposed mechanism.							
80 PAC/WIMI Neopentane Pyrolysis. P = (4-335) torr.	EX	823	2.2(9)			2	
$\text{CH}_3 + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_4\text{C}$							
Methyl + Ethyl, 1,1-dimethyl- (t-Butyl)							
76 MAR/PUR Estimated k. Computer-fit of data.	DE	756-845	7.9(12)	0	0	2	
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CHCH}_3$ (b)							
Methyl + Butane							
75 YAM k_a .	ES	980-1060	5.01(11)	0	6844	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 PAC/PUR1 ¹) Calculation based on experimental data.	DE	869-952	2.51(14)	0	9160±1610	2	6.31
74 HUG/MAR ¹) Calculation based on experimental data.	DE	895-981	3.16(13)	0	7434±1804	2	7.94
75 YAM ¹)	RN	980-1060	3.16(12)	0	5586±1007	2	2.57
76 YAM/NAM ¹) ¹) k _a + k _b .	EX	980-1060	3.16(12)	0	5586±1007	2	2.57
75 YAM k _b .	ES	980-1060	4.26(11)	0	5284	2	
CH ₃ + (CH ₃) ₃ CH → CH ₄ + (CH ₃) ₂ CHCH ₂ (a) → CH ₄ + (CH ₃) ₃ C (b)							
Methyl + Propane, 2-methyl- (i-Butyl)							
73 KON/MAR k _a .	ES	770-855	1.45(13)	0	8203	2	
82 SHE/GUS ¹) (k _a + k _b)/k _{ref} . Average ratio. k _{ref} :	RL	1023-1123	(2.2±0.2)				2/2
CH ₃ + CH ₃ CH ₂ CH ₃ → CH ₄ + CH ₃ CH ₂ CH ₂ (c) → CH ₄ + (CH ₃) ₂ CH (d)							
73 KON/MAR k _b .	ES	770-855	3.24(12)	0	6492	2	
82 SHE/GUS ¹) k _b /k _a . Recalculated from a reported tertiary per primary bond rate constant ratio of 10.5 ¹) Propane/Isobutane pyrolysis. P = 100 torr.	RL	1023-1123	1.17				2/2
CH ₃ + CH ₃ C(O)C(O)CH ₃ → (CH ₃) ₂ CO + CH ₃ CO (a) → CH ₄ + CH ₂ C(O)C(O)CH ₃ (b) → (CH ₃) ₂ C(O·)COCH ₃ (c)							
Methyl + 2,3-Butanedione (Biacetyl)							
73 KNO/SCH k _a . Estimation based on some experimental data.	ES	240-277	2.51(10)	0	3221	2	
75 SCH/PLA k _a .	RN	822-905	1.58(11)	0	4328	2	
73 KNO/SCH k _b . Estimation based on some experimental data.	ES	240-277	3.16(11)	0	4177	2	
75 SCH/PLA k _b .	RN	822-905	7.94(11)	0	4731	2	
75 SCH/PLA k _b /k _a .	RL	822-905	5.01	0	403±755	2	63.1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 SCH/KNO k_b/k_{ref} k_{ref} : $CH_3 + CD_3C(O)C(O)CD_3 \rightarrow CH_3D + CD_3C(O)C(O)CD_2$	RL	524-565	3.16	0	-302±428	2/2	3.16
78 KNO/SCH ¹⁾ k_b/k_c	RL	655-690	1.58(1)	0	1107±352	2/2	1.58
78 KNO/SCH ¹⁾ k_c	RN	655-690	2.0(10)	0	3070±503	2	2.51
¹⁾ Thermolysis. Gas-chromatography.							
$CH_3 + CD_3C(O)C(O)CD_3 \rightarrow CD_3CO + CH_3C(O)CD_3$ (a)							
$\rightarrow CD_3 + CH_3C(O)C(O)CD_3$ (b)							
$\rightarrow CH_3D + CD_2C(O)C(O)CD_3$ (c)							
Methyl + 2,3-Butanedione-1,1,1,4,4,4-d ₆ (Biacetyl-d ₆)							
77 SCH/KNO k_a/k_{ref} k_{ref} : $CD_3 + CD_3C(O)C(O)CD_3 \rightarrow CD_3CO + CD_3C(O)CD_3$	RL	524-565	5.0(-1)	0	604±403	2/2	2.51
77 SCH/KNO k_b/k_a	RL	524-565	3.16	0	3120±453	2/2	2.51
77 SCH/KNO k_c	RN	524-565	7.94(10)	0	7529±377	2	2.51
$CD_3 + CH_3C(O)C(O)CH_3 \rightarrow CD_3H + CH_2C(O)C(O)CH_3$							
Methyl-d ₃ + 2,3-Butanedione (Biacetyl)							
77 SCH/KNO k_{ref} : $CD_3 + CD_2HC(O)C(O)CD_3$ $\rightarrow CD_3H + CD_2C(O)C(O)CD_3$	RL	524-565	1.26	0	-906±101	2/2	1.26
$CD_3 + CD_2HC(O)C(O)CD_3 \rightarrow CD_2HC(O)D_3 + CD_3CO$							
Methyl-d ₃ + 2,3-Butanedione-1,1,1,4,4-d ₅ (Biacetyl-d ₅)							
77 SCH/KNO k_{ref} : $CD_3 + CD_3C(O)C(O)CD_3 \rightarrow CD_3CO + CD_3C(O)CD_3$	RL	660-685	2.0(-1)	0	-906±151	2/2	1.58
$CD_3 + CD_3C(O)C(O)CD_3 \rightarrow CD_4 + CD_2C(O)C(O)CD_3$ (a)							
$\rightarrow CD_3CO + (CD_3)_2CO$ (b)							
Methyl-d ₃ + 2,3-Butanedione-1,1,1,4,4,4-d ₆ (Biacetyl-d ₆)							
77 SCH/KNO k_a/k_{ref} k_{ref} : $CD_3 + CD_2HC(O)C(O)CD_3$ $\rightarrow CD_3H + CD_2C(O)C(O)CD_3$	RL	660-685	3.98	0	906±101	2/2	1.26
77 SCH/KNO k_a/k_b	RL	660-685	1.0(1)	0	1359±302	2/2	1.58

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 SCH/KNO k_a .	RN	660-685	1.26(11)	0	4680±377	2	2.51
77 SCH/KNO k_b .	RN	660-685	1.26(10)	0	3322±503	2	3.98
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_2$ (b) $\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{CHCH}_3$ (c) $\rightarrow (\text{CH}_3)_2\text{C}(\text{O}\cdot)\text{CH}_2\text{CH}_3$ (d)							
Methyl + 2-Butanone							
80 KNO ¹⁾ $(k_a + k_b + k_c)/k_d$.	RL	563	(4.95±1.90)(2)			2/2	
80 KNO ¹⁾ k_d .	RN	563	2.00(5)			2	2.51
¹⁾ Azomethane-sensitized decomposition.							
$\text{CH}_3 + \text{CD}_3\text{C}(\text{O})\text{CD}_2\text{CH}_3 \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{C}(\text{O})\text{CD}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{D} + \text{CD}_3\text{C}(\text{O})\text{CDCH}_3$ (b)							
Methyl + 2-Butanone-1,1,1,3,3-d ₅							
74 SCH/DRE $k_a + k_b$.	RN	523-563	1.26(11)	0	4504±277	2	2.58
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2$ (b) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CHCH}=\text{CH}_2$ (c) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2$ (d) $\rightarrow \text{CH}_4 + \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (e)							
Methyl + 1-Pentene							
74 SHI/AMA $(k_a + k_b)/(k_c + k_d + k_e)$.	RL	923	1.0			2/2	
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CHCH}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CHCH}_3$ (b) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_2$ (c) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CHCH}=\text{CHCH}_3$ (d) $\rightarrow \text{CH}_4 + \text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3$ (e)							
Methyl + 2-Pentene (Unspecified form)							
74 SHI/AMA $(k_a + k_b)/(k_c + k_d + k_e)$.	RL	923	2.0(-1)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{CH}_3)=\text{CH}_2$ (b) $\rightarrow \text{CH}_4 + \text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2$ (c)						
Methyl + 2-Butene, 2-methyl-						
75 BUL/MAR	ES	667-770	5.01(13)	0	7578	2
$k_a + k_b$. Static system pyrolysis.						
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$						
Methyl + Pentyl						
71 WAT	RL	298	$\geq 3.3(-1)$			2/2
Lower-limit estimate. k_{ref} : $\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CH}_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}_3$						
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (b)						
Methyl + Butyl, 1-methyl-						
71 WAT	RL	298	1.16			2/2
$(k_a + k_b)/k_a$.						
$\text{CH}_3 + (\text{CH}_3)_4\text{C} \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{CCH}_2$						
Methyl + Propane, 2,2-dimethyl- (Neopentane)						
71 MCN/KEL	RL	653	(6.7 ± 0.9)			2/2
k_{ref} : $\text{CH}_3 + \text{CD}_2=\text{C}=\text{O} \rightarrow \text{CH}_3\text{D} + \text{CD}=\text{C}=\text{O}$						
73 PAC	RN	793-953	3.16(13)	0	8059±241	2 1.26
76 BRA/WES1	DE	1030-1300	6.6(14)	0	10826	2 1.66
Computer data-fit to a proposed mechanism.						
72 FUR/LAI2	RN	529-608	4.9(11)	0	5788	2
Hg-photosensitized decomposition of Neopentane. k determined relative to the reaction: $\text{CH}_3 + \text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3$						
78 MAR/COM	EX	703-743	5.01(11)	0	5184	2
Stirred flow-reactor pyrolysis. P(Neopentane) = 50 torr.						
78 PAC/WIM	EX	821	$(1.36 \pm 0.16)(9)$			2
Neopentane flow-pyrolysis. P = 7.6 torr.						
80 PAC/WIM1	EX	823	$(1.6 \pm 0.1)(9)$			2
Pyrolysis of Neopentane in a flow-reactor. Gas-chromatography. P = (4-335) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{C}(\text{O})\text{CH}_2\text{CH}_3$ (a)							
$\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CHCH}_3$ (b)							
$\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_2\text{CH}_2$ (c)							
$\rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3\text{CH}_2\text{CO}$ (d)							
Methyl + 2,3-Pentanedione							
74 SCH/KNO k_b/k_a . T-dependence not detectable.	RL	362-398	≈ 4.5	0	0	2/2	
74 SCH/KNO k_c/k_a . T-dependence not detectable.	RL	362-398	$\approx 3.0(-1)$	0	0	2/2	
74 SCH/KNO $(k_a + k_b + k_c)/k_d$.	RL	362-398	2.51(1)	0	151±654	2/2	2.51
$\text{CH}_3 + \text{CH}_3\text{CD}_2\text{C}(\text{O})\text{CD}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_2\text{CD}_2\text{C}(\text{O})\text{CD}_2\text{CH}_3$ (a)							
$\rightarrow \text{CH}_3\text{D} + \text{CH}_3\text{CDC}(\text{O})\text{CD}_2\text{CH}_3$ (b)							
Methyl + 3-Pentanone-2,2,4,4-d ₄							
72 SCH/WOL1 k_a .	EX	513-572	2.00(11)	0	5544±454	2	3.16
72 SCH/WOL1 k_b .	EX	513-572	1.26(11)	0	4177±201	2	1.78
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (a)							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)_2\text{CH}_2$ (b)							
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CHC}(\text{CH}_3)=\text{CH}_2$ (c)							
$\rightarrow \text{CH}_4 + \text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (d)							
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(=\text{CH}_2)\text{CH}_2$ (e)							
Methyl + 1-Pentene, 2-methyl-							
74 SHI/AMA k_a/k_b .	RL	923	5.0			2/2	
74 SHI/AMA $(k_a + k_b)/(k_c + k_d + k_e)$.	RL	923	6.0(-1)			2/2	
$\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{CH}_3)_2$ (a)							
$\rightarrow \text{CH}_3\text{CH}_2\text{CHC}(\text{CH}_3)_3$ (b)							
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)\text{CH}_2$ (c)							
$\rightarrow \text{CH}_4 + \text{CH}_3\text{CHCH}=\text{C}(\text{CH}_3)_2$ (d)							
Methyl + 2-Pentene, 2-methyl-							
74 SHI/AMA k_a/k_b .	RL	923	1.0			2/2	
74 SHI/AMA $(k_a + k_b)/(k_c + k_d)$.	RL	923	1.2(-1)			2/2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3 + \text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_4\text{CH}_2$ (a)						
$\rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_3\text{CHCH}_3$ (b)						
$\rightarrow \text{CH}_4 + \text{CH}_3(\text{CH}_2)_2\text{CHCH}_2\text{CH}_3$ (c)						
Methyl + Hexane						
76 YAM	RN	973-1088	4.2(12)	0	5637	2
$k_a + k_b + k_c$.						
$\text{CH}_3 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}_2$ (a)						
$\rightarrow \text{CH}_4 + (\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2$ (b)						
Methyl + Butane, 2,3-dimethyl-						
75 BUL/MAR ¹⁾	RL	667-770	1.0(-1)	0	-2526	2/2
k_b/k_a . Estimated ratio.						
75 BUL/MAR ¹⁾	ES	667-770	2.00(13)	0	7217	2
$k_a + k_b$.						
¹⁾ Static system pyrolysis.						
$\text{CH}_3 + \text{CH}_3\text{C}(\text{O})\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$						
$\rightarrow \text{CH}_4 + \text{CH}_2\text{C}(\text{O})\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (a)						
$\rightarrow \text{CH}_4 + \text{CH}_3\text{C}(\text{O})\text{CHCH}_2\text{C}(\text{O})\text{CH}_3$ (b)						
$\rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (c)						
Methyl + 2,5-Hexanedione						
75 KNO/SCH	RL	515-712	1.0	0	-1631±10	2/2
$(k_a + k_b)/k_c$.						
75 KNO/SCH	CO	515-712	3.16(11)	0	4026	2
$k_a + k_b$.						
75 KNO/SCH	RN	515-712	3.16(11)	0	5637	2
k_c .						
$\text{CH}_3 + (\text{CH}_3)_3\text{COOC}(\text{CH}_3)_3 \rightarrow \text{CH}_4 + (\text{CH}_3)_3\text{COOC}(\text{CH}_3)_2\text{CH}_2$						
Methyl + Peroxide, bis(1,1-dimethylethyl)-						
80 KNO/RIC ¹⁾	RL	413	(3.5±0.3)			2/2
k_{ref} :						
$\text{CH}_3 + (\text{CD}_3)_2\text{CO} \rightarrow \text{CH}_3\text{D} + \text{CD}_2\text{C}(\text{O})\text{CD}_3$						
80 KNO/RIC ¹⁾	RN	413	(1.06±0.12)(6)			2
¹⁾ Thermolysis of Azomethane and di-t-Butylperoxide.						
Mass-spectrometry.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₄ (+ M) → CH₃ + H (+ M) (a)						
→ any other products (b)						
Methane						
71 DEA/KIS k _a . M = Ar. Shock-waves. Best-fit to experimental data. Total conc.: 5x10 ¹⁷ molec.cm ⁻³ .	DE	1750-2575	1.63(18)	0	51837	2
71 HAR/TRO k _a . M = Ar. Limiting high-pressure k.	EX	1850-2500	1.26(15)	0	52340±1007	1
71 HAR/TRO k _a . M = Ar. Low-pressure k.	EX	1850-2500	2.00(17)	0	44288±1007	2
72 NAP/SUB k _a . M = Ar.	EX	1750-2700	3.8(13)	0	47106	1
73 VOM2 k _a . M = Ne. The experimental conditions correspond to the limiting case of low pressures.	EX	2000-2700	3.98(9)	0	31706±2516	1 3.16
75 BOW1 k _a . M = Ar.	ES	1900-2400	1.4(17)	0	44500	2
75 CHE/BAC k _a . Limiting high-pressure k.	EX	995-1103	2.8(16)	0	54152	1
75 GAR/OWE k _a . M = H ₂ , Ne, Ar, Kr.	EX	2000-2700	2.3(14)	0	32477	2
75 ROT/JUS k _a . M = Ar.	EX	1700-2300	4.73(17)	0	46911	2
77 HEF/PAR k _a . M = Ar.	EX	2023-2721	2.2(17)	0	45345	2
78 PEN/SUL k _a . M = Ar. CH ₄ pyrolysis in reflected shock-waves. He/Ne Laser-absorption. P(Total) = (2.3-4.2) atm.	EX	2023-2721	2.2(17)	0	45345	2
79 TAB/BAU k _a . M = Ar. CH ₄ pyrolysis behind shock-waves. Total conc.: (1.4-5.4)x10 ¹⁸ molec.cm ⁻³ .	EX	1950-2770	(1.01±0.23)(17)	0	43181±503	2
80 ROT k _a . M = Ar. CH ₄ Thermolysis behind shock-waves. Atomic Resonance-Absorption Spectrophotometry. Same data published in 79 ROT/JUS1.	EX	1800-2300	4.73(17)	0	46800	2
82 KLO/DRO k _{overall} . M = Ar. CH ₄ pyrolysis behind single-pulse shock-waves. High-pressure. P = (6-10) atm.	EX	1500-3000	1.0(15)	0	51482	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CD₄ (+ M) → CD₃ + D (+ M)						
Methane-d ₄						
80 CHI/BAK ¹⁾	EX	1780-2440	1.4(11)	0	40765	1
80 CHI/BAK ¹⁾	EX	1780-2440	2.1(16)	0	42728	2
M = Ar.						
¹⁾ CD ₄ Pyrolysis behind shock-waves. Resonance-Absorption Spectroscopy.						
CHO (+ M) → CO + H (+ M)						
Methyl, oxo- (Formyl)						
76 TSU	DE	1500-2000	1.0(14)	0	11066	2
M = r. Computer calculation on the basis of a suggested mechanism.						
CHO + O₂ (+ M) → CO + HO₂ (+ M) (a)						
→ CO ₂ + OH (+ M) (b)						
→ HCO ₃ (+ M) (c)						
Methyl, oxo- (Formyl) + Oxygen molecule						
74 WAS/MAR	RL	297	(2.74±0.21)(-2)			2/2
k _a /k _{ref} . k _{ref} : O + CHO → H + CO ₂ (d) → OH + CO (e)						
81 MOR/HEI	RL	296	(2.1±0.7)(-1)			2/2
k _a /k _{ref} . Photolysis of NO ₂ in presence of HCHO and O ₂ , at 360 nm. P(Total) = 52 torr. k _{ref} : NO ₂ + CHO → NO + HCOO						
73 PEE/MAH1	ES	1600	≈3.0(13)			2
k _a . Tentative k.						
74 WAS/MAR	RN	297	(3.43±0.72)(12)			2
k _a . Ethylene used as source of CHO.						
76 MAR	RN	297	(4.70±2.59)(12)			2
k _a . Formaldehyde used as source of CHO.						
77 SHI/EBA	EX	298	(5.12±0.60)(12)			2
k _a .						
78 CLA/MOO	EX	298	(2.41±0.48)(12)			2
k _a . Monochromatic laser photolysis.						
78 REI/CLA	EX	298	(2.41±0.48)(12)			2
k _a . HCHO photolysis with tunable pulsed UV-laser.						
81 CHE/RHO	DE	250-2000	(3.5±0.5)(12)	0	0	2
k _a . Kinetic modelling of CO oxidation in flames.						
81 GIL/JOH	EX	298	(2.53±0.42)(12)			2
k _a . CH ₃ CHO Flash-photolysis. Time-resolved intracavity laser detection. P(CH ₃ CHO) = 0.2 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 VEY/LES k _a . CHO generated by Flash-photolysis of HCHO, or CH ₃ CHO. Laser-Resonance-absorption. The pre- exponential factor expressed as: A(T/298) ^{-0.4} . P(Total) = 45, or 500 torr.	EX	298-503	3.39(12)	-0.4	0	2
76 OSI/HEI k _b /k _a . Upper-limit ratio.	RL	296	≤1.9(-1)			2/2
79 NAD/SAR3 ¹⁾ k _b /k _a . Flash-photolysis of CH ₃ CHO, or HCHO. P(Total) = (13-100) torr.	RL	298	1.9(-1)			2/2
76 OSI/HEI k _c /k _{ref} . k _{ref} : CHO + O ₂ → CO + HO ₂	RL	296	(5.0±1.0)			2/2
79 NAD/SAR3 ¹⁾ k _c /k _a . Flash-photolysis of CH ₃ CHO, or HCHO. P(Total) = (13-100) torr.	RL	298	(5.0±1.0)			2/2
79 NAD/SAR3 ¹⁾ k _a + k _b + k _c . CH ₃ CHO flash-photolysis.	EX	298	(2.41±0.60)(12)			2
79 NAD/SAR3 ¹⁾ k _a + k _b + k _c . HCHO flash-photolysis.	EX	298	(2.23±0.48)(12)			2
¹⁾ Intracavity laser spectroscopy. P(Total) = (3-100) torr.						
78 HOR/SU k _c . HCHO photolysis at 313 nm. Lower-limit k. P(HCHO) = 8 torr. P(CO ₂) = (0-300) torr. P(O ₂) = (0.02-8) torr.	EX	298	≥(4.4±1.6)(17)			3
CHO + NO → CO + HNO						
Methyl, oxo- (Formyl) + Nitrogen oxide (NO)						
77 SHI/EBA	EX	298	(3.37±0.54)(12)			2
78 CLA/MOO Monochromatic laser photolysis.	EX	298	(8.73±1.20)(12)			2
78 REI/CLA HCHO photolysis with tunable pulsed UV-laser.	EX	298	(8.43±1.20)(12)			2
80 NAD/SAR CH ₃ CHO/HCHO/NO Flash-photolysis. Pulse-photolysis. Intracavity laser spectroscopy. P(Total) = (13-100) torr.	EX	298	(7.22±2.41)(12)			2
81 VEY/LES CHO generated by Flash-photolysis of HCHO, or CH ₃ CHO. Laser Resonance-absorption. P(Total) = 45, or 500 torr. The preexponential factor expressed as: A(T/298) ^{-0.4} .	EX	298-503	7.40(12)	-0.4	0	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
CHO + CH₃CH₂CH₂ → CO + CH₃CH₂CH₃ Methyl, oxo- (Formyl) + Propyl							
79 FOE/BER Butanal photolysis. k derived from a suggested reaction scheme.	DE	253-298	3.16(13)	0	0	2	1.58
CHO + CH₃CH₂CH₂CHOH → CO + CH₃CH₂CH₂CH₂OH Methyl, oxo- (Formyl) + Butyl, 1-hydroxy-							
79 FOE/BER Butanal photolysis. T-independent. Derived from a suggested reaction scheme. k_{ref} : CH ₃ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ CHOH → (CH ₃ CH ₂ CH ₂) ₂ CHOH	RL	253-298	(4.1±1.4)	0	0	2/2	
HCHO* (or HC(:)OH) → H + CHO (a) → H ₂ + CO (b)							
Formaldehyde (or Methylene, hydroxy-)							
79 MOR/HEI $k_a/(k_a + k_b)$. HCHO photolysis at 313 nm.	RL	296	(6.1±1.5)(-1)				1/1
HCHO (+ M) → H + CHO (+ M) (a) → H ₂ + CO (+ M) (b)							
Formaldehyde							
81 TSU/KAT ¹⁾ Total conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	ES	1500-1900	6.92(11)	0	36206	1	
81 TSU/KAT ¹⁾ Total conc. = 3.0x10 ¹⁹ molec.cm ⁻³ .	ES	1500-1900	2.51(12)	0	36206	1	
81 TSU/KAT ¹⁾ Total conc. = 6.0x10 ¹⁹ molec.cm ⁻³ .	ES	1500-1900	3.55(12)	0	36206	1	
¹⁾ k_a . M = Ar. CH ₃ OH/O ₂ thermal oxidation. Reflected shock-waves. UV-absorption.							
75 BOW1 k_a . M = Ar.	ES	1900-2400	1.0(14)	0	18500	2	
79 DEA/CRA k_a . M = Ar. Reflected shock waves. [HCHO] = (2.4-4.5)x10 ¹⁸ molec.cm ⁻³	EX	1800-2500	3.61(17)	0	43784±6014	2	2.95
80 DEA/JOH1 k_a . M = Ar. HCHO Decomposition behind shock-waves. Best data-fit. Total conc. = 5x10 ¹⁸ molec.cm ⁻³ .	EX	1700-2500	3.31(16)	0	40777	2	
73 PEE/MAH1 k_b . M = O ₂ , H ₂ O, CO ₂ .	EX	1100-1900	2.1(16)	0	17614±2516	2	
77 MIY/MOR k_b . Calculation based on a proposed mechanism.	DE	500-2090	2.1(15)	0	17620	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
81 VAN/VAN k_b . M = Ar. CH ₃ OH/O ₂ lean flames at 40 torr. Molecular beam sampling. Mass-spectrometry.	DE	1000-2000	2.5(14)	0	14595	2	
82 KLI/PEN k_b . M = H ₂ . HCHO/Ar Pyrolysis behind reflected shock-waves. P = (1.8-2.7) torr.	EX	1200-2200	2.4(13)	0	8254	2	
DCDO (+ M) → D + D + CO (+ M)							
Formaldehyde-d ₂							
80 CHI/SKI M = Ar. CD ₄ /O ₂ /Ar oxidation behind reflected shock-waves. Resonance-Absorption.	EX	1700-2200	4.5(16)	0	36206	2	
HCOOH (+ M) → CO + H₂O (+ M) (a) → CO₂ + H₂ (+ M) (b)							
Formic acid							
71 BLA/DAV ¹⁾ k_a .	EX	943-1053	2.45(12)	0	30432	1	
71 BLA/DAV ¹⁾ k_b . Static vessel.	EX	730-1053	2.95(9)	0	24417±854	1	2.95
71 BLA/DAV ¹⁾ k_b . Unpacked flow vessel.	EX	730-1053	2.75(8)	0	22962±349	1	1.48
71 BLA/DAV ¹⁾ k_b . Packed flow-vessel.	EX	730-1053	3.98(9)	0	26523±445	1	1.59
¹⁾ HCOOH Pyrolysis. Flow, or static system. P = (20-230) torr.							
76 SAM/PET ²⁾ Based on E _a (CHClF ₂) = (55.0±2.5) kcal.mol ⁻¹ .	EX	900-1000	3.16(14)	0	33216±1912	1	7.94
76 SAM/PET ²⁾ Based on E _a (CHClF ₂) = (55.8±2.5) kcal.mol ⁻¹ .	EX	900-1000	1.0(15)	0	33568±2013	1	7.94
76 SAM/PET ²⁾ Based on E _a (CHClF ₂) = (51.4±2.5) kcal.mol ⁻¹ .	EX	900-1000	3.16(13)	0	31052±1812	1	6.31
²⁾ $k_a + k_b$. Chanel (a) is predominant. HCOOH/CHClF ₂ Decomposition induced by a CO ₂ laser. P(HCOOH) = 1.5 torr. P(CHClF ₂) = 4 torr.							
82 HSU/SHA ³⁾ k_a . M = Ar.	EX	1280-2030	2.3(15)	0	25164±856	2	
82 HSU/SHA ³⁾ k_b .	EX	1280-2030	1.5(16)	0	28686±1409	2	
³⁾ M = Ar. HCOOH Pyrolysis behind incident, or reflected shock-waves. Laser-probing apparatus. P(Total) = (0.75-2.8) atm. [HCOOH] = (0.07-1.6)%							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
HCOOH + HCOOH → HCHO + CO₂ + H₂O						
Formic acid						
71 BLA/DAV HCOOH pyrolysis in a flow, or static system. Gas-chromatography. Above 873 K the Arrhenius plot becomes curved but straightens out again above 943 K, to become first order. P = (20-230) torr.	EX	730-873	2.75(11)	0	15938	2
CH₃O (+ M) → HCHO + H (+ M) (a) → CH₂OH (+ M) (b)						
Methoxy						
79 BAT k _a . Conventional static system.	ES	393-473	1.58(14)	0	13840±503	1 3.16
81 BAT/BUR k _b . Probably an upper-limit k.	ES	393-473	1.0(13)	0	13078±1151	1 3.16
82 GUT/SAN k _b . CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. M = N ₂ , or SF ₆ . P-independent. Upper-limit k. P = (10-100) torr.	ES	298	<2.0(2)			1
CH₃O* → HCHO + H						
Methoxy						
73 WIE/HEI M = N ₂ . k _{ref} : CH ₃ O* + M → CH ₃ O + M. CH ₃ O* formed by photolysis of CH ₃ ONO at 366 nm.	RL	298	1.04(-7)			1/2
CH₃O + O₂ → HCHO + HO₂						
Methoxy + Oxygen molecule						
73 WIE/VIL k _{ref} : CH ₃ O + NO → HCHO + HNO + CH ₃ ONO	RL	298	4.7(-5)			2/2
75 ALC/MIL	ES	373	1.2(9)			2
75 GLA k _{ref} : CH ₃ O + NO → CH ₃ ONO	RL	296	(5.2±0.7)(-5)			2/2
75 GLA Upper-limit ratio. k _{ref} : CH ₃ O + NO ₂ → CH ₃ ONO ₂	RL	296	≤(7.4±0.7)(-5)			2/2
75 MEN/GOL	ES	300	3.5(8)			2
77 ALC/MIL ¹⁾ Estimated ratio. k _{ref} : CH ₃ + (CH ₃) ₂ CHCH(CH ₃) ₂ → CH ₃ OH + (CH ₃) ₂ CHC(CH ₃) ₂	RL	373	(5.8±0.8)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A units	k err. factor
77 ALC/MIL ¹) Estimated ratio. k _{ref} : CH ₃ O ₂ + (CH ₃) ₂ CHCH(CH ₃) ₂ → CH ₃ OOH + (CH ₃) ₂ CHC(CH ₃) ₂	RL	373	3.3				2/2
77 ALC/MIL ¹) ¹) Azomethane photolysis.	ES	373	1.2(9)				2
77 BAR/BEN1 Vacuum technique. Chromatography.	RN	396-442	3.16(11)	0	2013±1409	2	31.6
79 BAT/RAT Static system. Gas-chromatography.	EX	383-433	1.0(12)	0	2265±554	2	4.0
79 BAT/ROB Static system. Gas-chromatography.	EX	383-433	1.0(12)	0	2416±554	2	4.0
80 COX/DER2 ONOC ₃ photolysis. Gas-chromatography.	EX	296-450	7.59(10)	0	1352±340	2	2.5
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced Fluorescence. Upper-limit k. P (Max) = 50 torr. Same data published in 80 SAN/BUT1.	EX	298	<1.20(9)				2
81 KIR/PAR Azo-t-butane/O ₂ photolysis. Upper-limit ratio. k _{ref} : CH ₃ O + (CH ₃) ₃ COOH → CH ₃ OH + (CH ₃) ₃ CO ₂	RL	373	<4.0(-1)				2/2
82 GUT/SAN CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. P(O ₂ + N ₂) = 40 torr.	EX	413-628	6.3(10)	0	1309	2	
CH₃O + O₃ → products							
Methoxy + Ozone							
75 SIM/HEI Upper-limit k.	EX	298	<1.20(9)				2
CH₃O + NO → HCHO + HNO (a) → CH₃ONO (b)							
Methoxy + Nitrogen oxide (NO)							
73 WIE/HEI ¹) Electronically excited ONOC ₃ .	RL	298-423	1.45(-1)	0	0		2/2
73 WIE/VIL ¹)	RL	298	1.45(-1)				2/2
75 GLA ¹) ¹) k _a /(k _a + k _b).	RL	296	1.3(-1)				2/2
75 BAT/MCC ²)	ES	393-473	3.98(12)	0	0±503	2	3.16
77 BAT/MIL3 ²) ²) k _a .	ES	440-473	2.0(12)	0	0±503	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 WIE/VIL ($k_a + k_b$)/ k_{ref} . k_{ref} : $CH_3O + NO_2 \rightarrow HCHO + HONO$ (c) $\rightarrow CH_3ONO_2$ (d)	RL	298	1.2				2/2
80 SAN/BUT2 $k_a + k_b$. M = SF ₆ . CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. Limiting high- pressure k. Same data given in 80 SAN/BUT1.	EX	298	(1.3±0.1)(13)				2
79 BAT/RAT k_b/k_{ref} . Static system. Spherical and packed reaction vessels. CH ₃ O generated by CH ₃ OOCH ₃ decomposition. k_{ref} : $CH_3O + NO_2 \rightarrow CH_3ONO_2$. [NO ₂] = (3.73-4.10)×10 ¹⁶ molec.cm ⁻³ . [NO] = (2.65-2.77)×10 ¹⁷ molec.cm ⁻³ . [CH ₃ OOCH ₃] = 6.0×10 ¹⁶ molec.cm ⁻³ .	RL	420	(2.03±0.47)				2/2
74 BAT/MIL ³)	ES	393-473	1.26(13)	0	0±503	2	2.51
75 BAT/MCC ³)	ES	393-473	1.26(13)	0	0±503	2	2.51
77 BAT/MIL3 ³) ³) k_b .	ES	440-473	1.26(13)	0	0±503	2	3.98
CH ₃ O + NO ₂ → HCHO + HONO (a) $\rightarrow CH_3ONO_2$ (b)							
Methoxy + Nitrogen oxide (NO ₂)							
77 BAR/BEN1 ¹) k_a/k_b . Assumed to be T-independent.	RL	396-442	(3.0±0.5)(-1)	0	0		2/2
77 BAR/BEN1 ¹) k_a . ¹) Vacuum technique. Chromatography.	RN	396-442	2.0(9)	0	0		2
77 BAT/MIL3 k_a .	ES	440-473	5.01(11)	0	0		2
73 WIE/VIL $k_b/(k_a + k_b)$.	RL	298	9.2(-1)				2/2
77 BAR/BEN1 k_b . Review of literature data.	SE	396-442	6.31(12)	0	0		2 3.16
77 BAT/MIL3 k_b .	ES	440-473	5.01(12)	0	0		2
79 BAT/RAT k_b . Static system. Spherical and packed reaction vessels. CH ₃ O generated by CH ₃ OOCH ₃ decomposition. [CH ₃ OOCH ₃] = 6.0×10 ¹⁶ molec.cm ⁻³ . [NO ₂] = (3.73-4.10)×10 ¹⁶ molec.cm ⁻³ . [NO] = (2.65-2.77)×10 ¹⁷ molec.cm ⁻³ .	RN	420	7.94(12)				2 2.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃O + N₂O → products							
Methoxy + Nitrogen oxide (N ₂ O)							
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. P(Max) = 5 torr. Upper-limit k.	EX	298	<1.20(10)			2	
CH₃O + NH₃ → CH₃OH + NH₂							
Methoxy + Ammonia							
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. P(Max) = 1 torr. Upper-limit k.	EX	298	<6.02(10)			2	
CH₃O + CO → CH₃ + CO₂ (a) → any other products (b)							
Methoxy + Carbon monoxide							
73 LIS/MAS k _a .	EX	396-426	1.6(13)	0	5939±755	2	3.98
73 WIE/HEI k _{overall} /k _{ref} . Assumed to be T-independent. k _{ref} : CH ₃ O + NO → HCHO + HNO (c) → CH ₃ ONO* (d)	RL	298-423	~5.0(-4)	0	0	2/2	
80 SAN/BUT2 k _{overall} . CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. Upper-limit k. P(Max) = 10 torr.	EX	298	<6.02(9)			2	
CH₃O + CH₄ → products							
Methoxy + Methane							
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. P(Max) = 10 torr. Upper-limit k.	EX	298	<6.02(9)			2	
CH₃O + CH₃O → HCHO + CH₃OH (a) → CH₃OOCH₃ (b)							
Methoxy							
73 SHO/HEI k _a /k _b .	RL	298	8.9			2/2	1.3
75 WEA/SHO ¹⁾ k _a /(k _a + k _b).	RL	288	1.0			2/2	
79 HAS/KOS k _a . Flash-photolysis of CH ₃ COOCH ₃ . Gas-chromatography. P = (1.5-700) torr.	EX	298	2.32(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
76 BAT/MCC1 k_b .	ES	383-413	2.0(13)	0	0	2	3.16
75 WEA/SHO ¹⁾ $k_b/(k_a + k_b)$.	RL	288	~0				2/2
¹⁾ Azomethane Photolysis.							
77 BAR/BEN2 k_b . VLP-Pyrolysis. RRKM best-fit estimate.	ES	391-432	5.01(12)	0	0	2	
CD₃O + CD₃O → DCDO + CD₃OD (a) → CD₃OCD₃ (b)							
Methoxy-d ₃							
75 WEA/SHO ¹⁾ $k_a/(k_a + k_b)$.	RL	288	1.0				2/2
75 WEA/SHO ¹⁾ $k_b/(k_a + k_b)$.	RL	288	~0				2/2
¹⁾ Azomethane-d ₆ Photolysis.							
CH₃O + CH₃OH → products							
Methoxy + Methanol							
80 SAN/BUT2 CH ₃ ONO photolysis at 266 nm. Laser-induced fluorescence. Upper-limit k. P(Max) = 1 torr. Same data given in SAN/BUT1.	EX	298	<6.02(10)				2
CH₃O + CH₂=CH₂ → CH₃OCH₂CH₂							
Methoxy + Ethene							
75 LIS/MAS	RN	300	(3.7±0.8)(7)				2
CH₃O + CH₃CO → HCHO + CH₃CHO							
Methoxy + Ethyl, 1-oxo- (Acetyl)							
79 HAS/KOS CH ₃ C(O)OCH ₃ Flash-photolysis. P = (1.5-700) torr.	EX	298	3.42(13)				2
CH₃O + CH₃CHO → CH₃OH + CH₃CO							
Methoxy + Acetaldehyde							
75 WEA/MEA Estimated ratio. k_{ref} : CH ₃ O + O ₂ → HCHO + HO ₂	RL	298	~(1.5±0.5)(1)				2/2
75 WEA/MEA	ES	298	(2.55±0.85)(9)				2
78 KEL/HEI ¹⁾ k_{ref} : CH ₃ O + O ₂ → HCHO + HO ₂	RL	298	(1.40±0.28)(1)				2/2
78 KEL/HEI ¹⁾	RN	298	(5.0±1.0)(9)				2
¹⁾ Azomethane photolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{O} + \text{CH}_3\text{OOCH}_3 \rightarrow \text{CH}_3\text{OH} + \text{HCHO} + \text{CH}_3\text{O}$ Methoxy + Peroxide, dimethyl-						
77 BAR/BEN1 Vacuum technique. Chromatography.	ES	391-432	$\approx 5.0(7)$	0	0	2
$\text{CH}_3\text{O} + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_3\text{COCH}_3$ Methoxy + Ethyl, 1,1-dimethyl- (t-Butyl)						
76 BAT/MCC1	ES	383-413	5.01(12)	0	0	2
$\text{CH}_3\text{O} + (\text{CH}_3)_3\text{CH} \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_3\text{C}$ Methoxy + Propane, 2-methyl-						
79 BAT/RAT Static system.	EX	383-433	3.98(11)	0	1208 \pm 554	2 3.98
80 SAN/BUT2 CH_3ONO photolysis at 266 nm. Laser-induced Fluorescence. Upper-limit k. P(Max) = 0.5 torr. Same data given in 80 SAN/BUT1.	EX	298	<1.20(11)			2
$\text{CH}_3\text{O} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{products}$ Methoxy + 1-Butene						
80 SAN/BUT2 CH_3ONO photolysis at 266 nm. Laser-induced Fluorescence. Upper-limit k. P(Max) = 0.25 torr. Same data given in 80 SAN/BUT1.	EX	298	<2.41(11)			2
$\text{CH}_3\text{O} + (\text{CH}_3)_3\text{COOH} \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_3\text{CO}_2$ Methoxy + Hydroperoxide, 1,1-dimethylethyl- (t-Butyl hydroperoxide)						
81 KIR/PAR Azo-t-butane/ O_2 Photolysis. Lower-limit k, determined relative to reaction: $\text{CH}_3\text{O} + \text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2$	RN	373	>4.22(9)			2
$\text{CH}_3\text{O} + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_2\text{CCH}(\text{CH}_3)_2$ Methoxy + Butane, 2,3-dimethyl-						
75 ALC/MIL	ES	373	4.0(8)			2
$\text{CH}_2\text{OH} (+ \text{M}) \rightarrow \text{HCHO} + \text{H} (+ \text{M})$ Methyl, hydroxy-						
75 BOW2 M = Ar. Reflected shock waves. Best data-fit. [Ar] = (5.7-17.0) $\times 10^{18}$ molec.cm ⁻³ . [CH ₂ OH] = 1.3 $\times 10^{17}$ molec.cm ⁻³ .	ES	1545-2180	3.0(9)	0	14600	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 TSU/KAT ¹) Total conc. = 6.0×10^{18} molec.cm ⁻³ .	CO	1500-1900	1.3(10)	0	14550	1
81 TSU/KAT ¹) Total conc. = 3.0×10^{19} molec.cm ⁻³ .	CO	1500-1900	5.6(10)	0	14550	1
81 TSU/KAT ¹) Total conc. = 6.0×10^{19} molec.cm ⁻³ .	CO	1500-1900	1.0(11)	0	14550	1
¹) M = Ar. CH ₃ OH/O ₂ thermal oxidation in Ar, behind reflected shock-waves. Same data given in 81 TSU/HAS.						
CH₂OH + O₂ → HCHO + HO₂						
Methyl, hydroxy- + Oxygen molecule						
80 RAD M = He. Flow-tube. LMR-spectroscopy. P(He) = 0.5 torr.	EX	300	1.20(12)			2 2.0
81 TSU/HAS M = Ar. CH ₃ OH/O ₂ thermal oxidation behind reflected shock-waves.	ES	1200-1800	1.0(13)	0	0	2
81 VAN/VAN CH ₃ /O ₂ oxidation in lean flames. Molecular beam sampling. Mass-spectrometry. P = 40 torr.	DE	1000-2000	1.0(14)	0	2516	2
CH₂OH + H₂O → CH₃OH + OH						
Methyl, hydroxy- + Water						
81 TSU/HAS M = Ar.	CO	1200-1800	1.55(14)	0	13231	2
CH₂OH + H₂O₂ → CH₃OH + HO₂						
Methyl, hydroxy- + Hydrogen peroxide						
81 TSU/HAS M = Ar.	CO	1200-1800	2.69(11)	0	-241	2
CH₃O₂ + O₃ → products						
Methyldioxy + Ozone						
75 SIM/HEI Upper-limit k.	EX	298	<1.45(7)			2
CH₃O₂ + SO₂ → CH₃O + SO₃ (a) → CH₃O₂SO₂ (b)						
Methyldioxy + Sulfur dioxide						
78 WHI/BOT k _a . Kinetic spectroscopy. Upper-limit k.	EX	298	≤2.0(9)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 SIM/HEI k_b/k_{ref} . Azomethane/O ₂ /SO ₂ /NO photolysis. k_{ref} : CH ₃ O ₂ + NO → CH ₃ O + NO ₂ .	RL	296	(2.5±0.5)(-3)			2/2
81 KAN/CAL k_b . Azomethane/SO ₂ /Air photolysis. FTIR-Spectroscopy. P(O ₂) = 100 torr. P(N ₂) = 600 torr.	EX	298	(8.43±1.20)(9)			2
79 KAN/MCQ ¹⁾	ES	298	≤(3.2±0.7)(9)			2
79 KAN/MCQ ¹⁾	ES	298	≤(6.4±1.4)(9)			2
¹⁾ $k_a + k_b$. Azomethane/Oxygen Flash-photolysis. k estimated as 1/2 of the measured apparent k. The lower limit estimate probably most nearly correct.						
79 SAN/SIM $k_a + k_b$. Flash-photolysis of Cl ₂ /CH ₄ /O ₂ mixtures. P = (60-700) torr.	EX	298	(4.94±0.30)(9)			2
81 SAN/WAT1 $k_a + k_b$. CH ₃ O ₂ produced by Cl ₂ /CH ₄ /O ₂ Photolysis. UV-Absorption. Upper-limit k. [CH ₃ O ₂] ₀ = (0.5-5.0)×10 ¹² molec.cm ⁻³ . [SO ₂] = (0.76-5.66)×10 ¹⁶ molec.cm ⁻³ . P(Total) ~250 torr.	EX	298-423	≤3.01(7)			2
CH ₃ O ₂ + NO → CH ₃ O + NO ₂ (a) → CH ₃ O ₂ NO (b) → HCHO + HONO (c)						
Methyldioxy + Nitrogen oxide (NO)						
74 SIM/HEI3 $k_a/(k_a + k_b)$.	RL	298	2.2			2/2
76 COX/DER2 k_a . Lower-limit estimate.	ES	298	≥7.23(11)			2
79 SIM/HEI k_a . Azomethane/O ₂ /SO ₂ /NO photolysis. Determined relative to the reaction: SO ₂ + CH ₃ O ₂ → CH ₃ O ₂ SO ₂ .	RN	296	1.90(12)			2 1.58
80 COX/TYN k_a . Molecular modulation-UV Absorption spectroscopy. P = 540 torr.	EX	298	(3.91±1.20)(12)			2
80 SAN/WAT k_a . Flash-photolysis. UV-absorption. P = (50-700) torr.	EX	298	(4.28±0.84)(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PLU/RVA1 k _a . M = He. Discharge-flow. Mass-spectrometry. CH ₃ O ₂ generated by reacting Cl atom with CH ₄ in presence of O ₂ . [Cl] ₀ = (2.0-7.0)x10 ¹¹ molec.cm ⁻³ . [O ₂] = (8.0-10.0)x10 ¹⁵ molec.cm ⁻³ . [NO] = (0.25-3.0)x10 ¹³ molec.cm ⁻³ . [He] = 1.9x10 ¹⁷ molec.cm ⁻³ .	EX	295	(5.18±1.20)(12)			2
81 SIM/HEI k _a . M = CH ₄ . Flash-photolysis of Cl ₂ in presence of CH ₄ /O ₂ /NO mixtures. UV-Absorption spectroscopy. P(Total) ~ 200 torr. P(CH ₃ O ₂) ₀ = (0.7-2.0) torr. P(NO) ₀ = (11-28) mtorr. P(CH ₄) = (70-600) torr.	EX	218-365	(1.26±0.60)(12)	0	-380±250	2
73 SPI/VIL k _b /(k _a + k _b).	RL	298	(6.0±1.0)(-1)			2/2
78 ANA/SMI2 k _a + k _b + k _c . Flash-photolysis of Azomethane/O ₂ /NO mixtures. Lower-limit k. [Azomethane] = (1.0-3.0)x10 ¹⁷ molec.cm ⁻³ . [NO] = (0.1-1.0)x10 ¹⁶ molec.cm ⁻³ .	ES	298	>6.02(11)			2
79 ADA/BAS1 k _a + k _b + k _c . Flash-photolysis. Kinetic spectroscopy. [Azomethane] = 5.5x10 ¹⁶ molec.cm ⁻³ . [O ₂] = 7.2x10 ¹⁶ molec.cm ⁻³ . [Ar] ~ 2.4x10 ¹⁸ molec.cm ⁻³ .	EX	298	(1.8±0.1)(12)			2
79 PLU/RVA k _a + k _b + k _c . Flow-reactor. Mass-spectrometry. Channel (a) is predominant.	EX	295	(4.82±1.20)(12)			2
81 RAV/EIS ¹⁾	EX	240-339	(3.79±1.51)(12)	0	-86±112	2
81 RAV/EIS ¹⁾	EX	240-339	(4.88±0.96)(12)	0	0	2
Nearly T-independent k (E _a ~0 preferred).						
¹⁾ k _a + k _b + k _c . Azomethane (or Cl ₂)/O ₂ pulsed laser-photolysis in Ar(or CH ₄) at 355 nm. Laser-induced Fluorescence. Channel (a) predominant. P(Ar) = (40-100) torr. P(CH ₄) = 50 torr. [Azomethane] = (0.5-1.6)x10 ¹⁶ molec.cm ⁻³ . [CH ₃ O ₂] = (1.2-8.6)x10 ¹² molec.cm ⁻³ . [O ₂] = (1.2-2.6)x10 ¹⁷ molec.cm ⁻³ . [NO] = (0.7-4.1)x10 ¹⁴ molec.cm ⁻³ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{O}_2 + \text{NO}_2 \rightarrow \text{CH}_3\text{O} + \text{NO}_3$ (a)						
$\rightarrow \text{HCHO} + \text{HONO}_2$ (b)						
$\rightarrow \text{CH}_3\text{OONO}_2$ (c)						
Methyldioxy + Nitrogen oxide (NO_2)						
76 COX/DER2 ($k_a + k_b + k_c$)/ k_{ref} . Approximate ratio. k_{ref} : $\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{O} + \text{NO}_2$	RL	298	$\approx 5.0(-2)$			2/2
80 ADA/BAS1 $k_a + k_b + k_c$. Azomethane Flash-photolysis. Kinetic Spectroscopy. P = (53-580) torr.	EX	298	$(9.2 \pm 0.4)(11)$			2
73 SPI/VIL $k_c/(k_b + k_c)$.	RL	298	$(7.5 \pm 0.5)(-1)$			2/2
80 COX/TYN ¹⁾ P(N_2) = 540 torr.	EX	298	$(9.6 \pm 1.81)(11)$			2
80 COX/TYN ¹⁾ P(Ar + CH_4) = 50 torr.	EX	298	$(7.23 \pm 1.81)(11)$			2
¹⁾ k_c . UV-Absorption Spectroscopy.						
80 RAV/EIS ²⁾ P(N_2) = 76 torr.	EX	298	$(8.19 \pm 1.39)(11)$			2
80 RAV/EIS ²⁾ P(N_2) = 722 torr.	EX	298	$(2.48 \pm 0.23)(12)$			2
²⁾ k_c . M = N_2 . Azomethane/ $\text{N}_2/\text{O}_2/\text{NO}_2$ photolysis. k's at other temperatures, for various N_2 pressures and concentrations of reactants also included. [Azomethane] = (0.5-2.1) molec.cm ⁻³ . [CH_3O_2] ₀ = (0.9-0.7) molec.cm ⁻³ . [NO_2] = (2.6-31.7) molec.cm ⁻³ .						
80 SAN/WAT ³⁾ M = He.	EX	298	$(5.32 \pm 0.39)(11)$			2
80 SAN/WAT ³⁾ M = N_2 .	EX	298	$(6.93 \pm 0.60)(11)$			2
80 SAN/WAT ³⁾ M = SF_6 .	EX	298	$(7.71 \pm 0.96)(11)$			2
³⁾ k_c . Flash-photolysis/UV-Absorption. P = 50 torr. Other k's are given for various pressures up to to 700 torr. The k's increase with the pressure.						
$\text{CH}_3\text{O}_2 + \text{CO} \rightarrow \text{CH}_3\text{O} + \text{CO}_2$						
Methyldioxy + Carbon monoxide						
80 SAN/WAT Flash-photolysis/UV-Absorption. P = (50-700) torr. Upper-limit k.	EX	298	$\leq 4.22(6)$			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃O₂ + HCHO → CH₃OOH + CHO						
Methyldioxy + Formaldehyde						
79 SEL/WAD Di-t-butyl peroxide pyrolysis in a static system.	ES	410	≈1.2(6)			2
CH₃O₂ + CH₃O₂ → HCHO + CH₃OH + O₂ (a)						
→ CH ₃ O + CH ₃ O + O ₂ (b)						
→ CH ₃ OOCH ₃ + O ₂ (c)						
Methyldioxy						
75 ALC/MIL k _a .	ES	373	2.4(11)			2
75 PAR k _a . Unreported T assumed to be 298 K.	EX	298	1.48(11)			2
77 ALC/MIL k _a . Azomethane photolysis.	RN	373	2.4(11)			2
77 ALC/MIL k _a /k _b . Estimated ratio. Azomethane photolysis.	RL	373	(2.5±1.2)(-1)			2/2
79 SEL/WAD k _a /k _b . Di-t-butyl peroxide thermolysis. Static system. Gas-chromatography. Mass-spectrometry.	RL	410	(6.9±0.8)(-1)			2/2
80 KAN/CAL ¹⁾ k _a /k _b .	RL	298	(1.32±0.16)			2/2
80 KAN/CAL ¹⁾ k _a /k _c . Lower-limit ratio.	RL	298	≥7.0			2/2
¹⁾ Photolysis of Azomethane and Oxygen mixtures.						
75 WEA/MEA ²⁾	RL	298	5.0(-1)			2/2
75 WEA/SHO ²⁾ Azomethane photolysis. FTIR-Spectroscopy.	RL	288	5.0(1)			2/2
81 NIK/MAK ²⁾ Photooxidation of Azomethane, or Cl-atom initiated oxidation of CH ₄ in O ₂ /N ₂ . FTIR-method. P = 700 torr.	RL	297	6.0(-1)			2/2
²⁾ k _a /(k _a + k _b + k _c).						
75 ALC/MIL ³⁾	ES	373	2.3(11)			2
75 PAR ³⁾	EX	298	8.73(10)			2
77 ALC/MIL ³⁾ Azomethane photolysis.	ES	373	2.3(11)			2
77 PAR ³⁾ ³⁾ k _b .	EX	298	(9.64±2.41)(10)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 WEA/MEA ⁴⁾	RL	298	4.3(-1)			2/2
75 WEA/SHO ⁴⁾	RL	288	4.3(-1)			2/2
Azomethane photolysis.						
81 NIK/MAK ⁴⁾	RL	297	3.2(-1)			2/2
Photooxidation of Azomethane, or Cl-atom, initiated oxidation of CH ₄ in O ₂ /N ₂ . FTIR-method. P = 700 torr.						
⁴⁾ k _b /(k _a + k _b + k _c).						
75 WEA/MEA ⁵⁾	RL	298	7.0(-2)			2/2
75 WEA/SHO ⁵⁾	RL	288	7.2(-2)			2/2
Azomethane Photolysis.						
81 NIK/MAK ⁵⁾	RL	297	8.0(-2)			2/2
Photooxidation of Azomethane, or Cl-atom initiated oxidation of CH ₄ in O ₂ /N ₂ . FTIR-method. P = 700 torr.						
⁵⁾ k _c /(k _a + k _b + k _c).						
75 PAR ⁶⁾	EX	298	(2.35±0.30)(11)			2
79 COX/TYN ⁶⁾	EX	298	(3.13±0.54)(11)			2
⁶⁾ k _a + k _b .						
77 PAR	EX	298	(1.84±0.48)(11)			2
k _a + k _c .						
73 PAR/PAU ⁷⁾	EX	298	(1.99±0.66)(11)			2
77 HOC/GHO ⁷⁾	EX	295	(2.3±0.3)(11)			2
Molecular-Modulation UV-Absorption Spectrometry.						
78 ANA/SMI2 ⁷⁾	EX	298	(2.65±0.60)(11)			2
Azomethane/O ₂ Flash-photolysis. [Azomethane] = (1-3)×10 ¹⁷ molec.cm ⁻³ .						
79 KAN/MCQ ⁷⁾	ES	298	(2.4±0.1)(11)			2
Azomethane/O ₂ Flash-photolysis.						
79 SAN/SIM ⁷⁾	EX	298	(2.23±0.18)(11)			2
Flash-photolysis of Cl ₂ /CH ₄ /O ₂ . P = (70-600) torr.						
80 ADA/BAS2 ⁷⁾	EX	298	(3.5±0.3)(11)			2
Azomethane/O ₂ Flash-photolysis.						
80 SAN/WAT ⁷⁾	EX	298	(2.17±0.42)(11)			2
Flash-photolysis. UV-Absorption. P = (50-700) torr.						
81 SAN/WAT2 ⁷⁾	EX	248-417	(8.43±1.20)(10)	0	-223±41	2
CH ₃ O ₂ produced by Cl ₂ /CH ₄ /O ₂ Flash-photolysis. UV-Absorption Spectrometry. [CH ₃ O ₂] = (0.04-2.0)×10 ¹⁴ molec.cm ⁻³ . P(Total) ~ 250 torr.						
⁷⁾ k _a + k _b + k _c .						

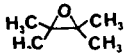
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CD}_3\text{O}_2 + \text{CD}_3\text{O}_2 \rightarrow \text{DCDO} + \text{CD}_3\text{OD} + \text{O}_2$ (a)						
$\rightarrow \text{CD}_3\text{O} + \text{CD}_3\text{O} + \text{O}_2$ (b)						
$\rightarrow \text{CD}_3\text{OCCD}_3 + \text{O}_2$ (c)						
Methyldioxy-d ₃						
75 WEA/MEA ¹) ⁴)	RL	298	4.1(-1)			2/2
75 WEA/SHO ¹) ⁴)	RL	288	6.0(-1)			2/2
¹) $k_a/(k_a + k_b + k_c)$.						
75 WEA/MEA ²) ⁴)	RL	298	4.5(-1)			2/2
75 WEA/SHO ²) ⁴)	RL	288	2.2(-1)			2/2
²) $k_b/(k_a + k_b + k_c)$.						
75 WEA/MEA ³) ⁴)	RL	298	1.4(-1)			2/2
75 WEA/SHO ³) ⁴)	RL	288	1.8(-1)			2/2
³) $k_c/(k_a + k_b + k_c)$.						
⁴) Azomethane-d ₆ Photolysis.						
$\text{CH}_3\text{O}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{O} + \triangle^{\text{O}}$						
Methyldioxy + Ethene						
80 SEL/WAD	EX	410	(1.2±0.7)(3)			2
Di-t-Butyl peroxide oxidation.						
Static system.						
Gas-chromatography.						
Mass-spectrometry.						
81 NIK/MOS	EX	593	(4.6±0.9)(7)			2
CH ₃ O ₂ generated by Thermolysis of Di-t-butyl peroxide [P(Total) = (50-400) torr.], or of Azomethane [P(Total) = (50-60) torr.], in presence of O ₂ and CH ₂ =CH ₂ .						
Gas-chromatography.						
$\text{CH}_3\text{O}_2 + \text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow \text{CH}_3\text{O} + \text{CH}_3 + \text{CO}_2 + \text{O}_2$						
Methyldioxy + Ethyldioxy, 1-oxo-						
80 ADD/BURR	DE	302	1.81(12)			2 2.0
Cl ₂ modulated photolysis, in presence of CH ₃ CHO and O ₂ .						
Computer simulation data-fit.						
$\text{CH}_3\text{O}_2 + \text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{products (overall)}$						
Methyldioxy + Diazene, dimethyl- (Azomethane)						
79 KAN/MCQ	EX	298	(8.0±3.0)(7)			2
Azomethane/O ₂ Flash-photolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{CHO}_2 \rightarrow \text{CH}_3\text{OH} + (\text{CH}_3)_2\text{CO} + \text{O}_2$ Methyldioxy + Ethyldioxy, 1-methyl-						
77 ALC/MIL Azomethane photolysis. Same data given in 75 ALC/MIL.	ES	373	6.2(11)			2
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_3\text{O} + \begin{array}{c} \text{O} \\ \diagup \quad \diagdown \\ \text{CH}_2 \quad \text{CH}_2 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ Methyldioxy + 1-Propene, 2-methyl-						
80 SEL/WAD Di-t-Butyl peroxide oxidation. Static system. Gas-chromatography. Mass-spectrometry.	EX	410	(9.8±1.6)(3)			2
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_3\text{CO}_2 \rightarrow \text{CH}_3\text{O} + (\text{CH}_3)_3\text{CO} + \text{O}_2$ (a) $\rightarrow \text{HCHO} + (\text{CH}_3)_3\text{OH} + \text{O}_2$ (b) Methyldioxy + Ethyldioxy, 1,1-dimethyl-						
75 PAR $k_a = k_b$. Unreported T assumed to be 298 K.	EX	298	(3.01±1.51)(10)			2
81 KIR/PAR ¹⁾	EX	333	1.0			2
81 KIR/PAR ¹⁾	EX	373	1.7			2
¹⁾ k_a/k_b . Azo-t-butane/O ₂ photolysis. Gas-chromatography. Approximate rate ratios.						
$\text{CH}_3\text{O}_2 + \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{O} + \begin{array}{c} \text{O} \\ \diagup \quad \diagdown \\ \text{CH}_2 \quad \text{CH}_2 \\ \quad \\ \text{CH}_3 \quad \text{CH}_3 \end{array}$ Methyldioxy + 1-Butene, 2-methyl-						
80 OSB/WAD Di-t-Butyl peroxide oxidation. Static system. Gas-chromatography. Mass-spectrometry.	EX	373-403	3.98(11)	0	6351±650	2 5.25
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{C}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{O} + \begin{array}{c} \text{H}_3\text{C} \quad \text{O} \\ \diagup \quad \diagdown \\ \text{C} \quad \text{C} \\ \quad \\ \text{H}_3\text{C} \quad \text{CH}_3 \end{array}$ Methyldioxy + 2-Butene, 2-methyl-						
80 OSB/WAD Di-t-Butyl peroxide oxidation. Static system. Gas-chromatography. Mass-spectrometry.	EX	373-403	1.44(11)	0	5100±433	2 3.09

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{O} + $ 							
Methylidioxy + 2-Butene, 2,3-dimethyl- 80 OSE/WAD Di-t-Butyl peroxide oxidation. Static system. Gas-chromatography. Mass-spectrometry.	EX	373-403	1.38(11)	0	4378±337	2	2.09
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OOH} + (\text{CH}_3)_2\text{C}(\text{CH}_3)_2$							
Methylidioxy + Butane, 2,3-dimethyl- 75 ALC/MIL 77 ALC/MIL Azomethane photolysis.	ES	373	1.6(5)			2	
$\text{CH}_3\text{O}_2 + (\text{CH}_3)_2\text{C}(\text{OO}\cdot)(\text{CH}_3)_2$ $\rightarrow \text{HCHO} + (\text{CH}_3)_2\text{C}(\text{OH})(\text{CH}_3)_2 + \text{O}_2$							
Methylidioxy + Propylidioxy, 1,1,3-trimethyl- 77 ALC/MIL Azomethane photolysis.	ES	373	2.4(11)			2	
$\text{HOCH}_2\text{O} + \text{O}_2 \rightarrow \text{HCOOH} + \text{HO}_2$							
Methoxy, hydroxy- + Oxygen molecule 82 VEY/RAY HCHO/O ₂ /NO Flash-photolysis. Computer simulation data-fit. [HCHO] ₀ = (2-30) torr. [O ₂] ₀ = (2.5-45) torr. [NO] ₀ = (15-200) torr.	DE	298	(2.11±0.96)(10)			2	
$\text{HOCH}_2\text{O} + \text{NO} \rightarrow \text{HOCH}_2\text{ONO}$ (a) $\rightarrow \text{HNO} + \text{HCOOH}$ (b)							
Methoxy, hydroxy- + Nitrogen oxide (NO) 82 VEY/RAY k _a + k _b . HCHO/O ₂ /NO flash-photolysis. Computer simulation data-fit. [O ₂] ₀ = (2.5-45) torr. [HCHO] ₀ = (2-30) torr. [NO] ₀ = (15-200) torr.	DE	298	(2.41±1.14)(13)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
HOCH₂O₂ + HO₂ + HCHO						
Methylldioxy, hydroxy-						
79 SU/CAL3 Cl ₂ /HCHO/synthetic air photolysis. FTIR-Spectroscopy. P(Total) ~ 700 torr.	ES	298	1.5			1
82 VEY/RAY HCHO/O ₂ /NO flash-photolysis. Data-fit. [O ₂] ₀ = (2.5-45) torr. [NO] ₀ = (15-200) torr. [HCHO] ₀ = (2-30) torr.	ES	298	3.0(1)			1
HOCH₂O₂ + NO → HOCH₂O + NO₂						
Methylldioxy, hydroxy- + Nitrogen oxide (NO)						
82 VEY/RAY HCHO/O ₂ /NO flash-photolysis. Data-fit. [O ₂] ₀ = (2.5-445) torr. [NO] ₀ = (15-200) torr. [HCHO] ₀ = (2-30) torr.	ES	298	3.37(12)			2
HOCH₂O₂ + HOCH₂O₂ → HOCH₂O + HOCH₂O + O₂						
Methylldioxy, hydroxy-						
79 SU/CAL3 Cl ₂ /HCHO/synthetic air photolysis. FTIR-Spectroscopy. P(Total) ~ 700 torr.	ES	298	7.23(10)			2
CH₃OH (+ M) → CH₃ + OH (+ M)						
Methanol						
75 BOW2 M = Ar. Reflected shock waves. Best data-fit. [Ar] = (5.7-17.0)x10 ¹⁸ molec.cm ⁻³ . [CH ₃ OH] = 1.3x10 ¹⁷ molec.cm ⁻³ . [O ₂] = 2.5x10 ¹⁷ molec.cm ⁻³ .	ES	1545-2180	4.0(15)	0	34200	2
81 TSU/KAT ¹) Total conc. = 6.0x10 ¹⁸ molec.cm ⁻³ .	EX	1500-1900	6.0(12)	0	37288	1
81 TSU/KAT ¹) Total conc. = 3.0x10 ¹⁹ molec.cm ⁻³ .	EX	1500-1900	3.5(13)	0	37769	1
81 TSU/KAT ¹) Total conc. = 6.0x10 ¹⁹ molec.cm ⁻³ .	EX	1500-1900	8.7(13)	0	38251	1
81 TSU/KAT ¹) Limiting high-pressure k. Tentative.	EX	1500-1900	2.0(18)	0	47510	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 TSU/KAT ¹⁾ Limiting low-pressure k. Tentative.	EX	1500-1900	9.0(18)	0	40536	2	
¹⁾ M = Ar. CH ₃ /O ₂ Thermal oxidation behind reflected shock-waves. UV-absorption. IR-emission. Same data given in 81 TSU/HAS.							
82 SPI/WAG ²⁾ Limiting high-pressure k.	EX	1600-2100	9.4(15)	0	45227	1	
82 SPI/WAG ²⁾ Limiting low-pressure k.	EX	1600-2100	2.0(17)	0	34441	2	
²⁾ Methanol Thermolysis behind reflected shock-waves. Total conc. = (0.1-3.8)x10 ¹⁹ molec.cm ⁻³ . [CH ₃ OH] ₀ = (0.1-3.0)x10 ¹⁶ molec.cm ⁻³ .							
CS₂ (+ M) → CS + S (+ M)							
Carbon disulfide							
74 TRA ¹⁾ Shock-tube. Unspecified high-T range.	EX	¹⁾	6.76(14)	0	35984±705	2	
80 SAI/TOR M = Ar. Thermolysis behind reflected shock-waves. [CS ₂] = (0.9-2.4)x10 ¹⁶ molec.cm ⁻³ . Total Conc. = (2.0-4.8)x10 ¹⁶ molec.cm ⁻³ .	EX	2000-2900	2.51(14)	0	37393±3271	2	3.16
COS (+ M) → products							
Carbon oxide sulfide							
74 TRA ¹⁾ Shock-tube. Unspecified high-T range.	EX	¹⁾	8.32(14)	0	31706±654	2	
CH₃S + CH₃S → HCS + CH₃SH (a) → CH₃SSCH₃ † (b)							
Methylthio							
73 TYC/KNI ¹⁾ k _a /k _b .	RL	298	4.0(-2)				2/2
73 TYC/KNI ¹⁾ k _a .	RN	298	9.8(11)				2
73 TYC/KNI ¹⁾ k _b .	RN	298	2.4(13)				2
¹⁾ Hg-photosensitized CH ₃ SH decomposition.							
CH₃S + #172 → CH₃S₂ + CH₂=CH₂							
Methyl, mercapto- + Thirane (Ethylene episulfide)							
72 JAK/AHM	ES	304-478	~3.16(11)	0	~4429	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
CN (+ M) → C + N (+ M)							
Cyanogen							
76 SLA M = Ar.	EX	4400-1300	(1.2±0.4)(14)	0	70961±5536	2	
CN(v=n) + O₂ → NCO + O							
Cyanogen + Oxygen molecule							
72 BUL/COO1 ¹⁾ v = 0.	EX	303	(6.77±0.15)(12)			2	
72 BUL/COO1 ¹⁾ v = 0.	EX	375	(6.34±0.22)(12)			2	
72 BUL/COO1 ¹⁾ v = 1.	EX	303	(7.6±0.2)(12)			2	
72 BUL/COO1 ¹⁾ v = 2.	EX	303	(9.26±0.22)(12)			2	
72 BUL/COO1 ¹⁾ v = 3.	EX	303	(9.83±0.31)(12)			2	
72 BUL/COO1 ¹⁾ v = 4.	EX	303	(1.17±0.35)(13)			2	
72 BUL/COO1 ¹⁾ v = 4.	EX	375	(1.11±0.06)(13)			2	
¹⁾ Possible small negative E _a .							
72 SCH/WOL2 k decreasing to 1.8x10 ¹² cm ³ mol ⁻¹ s ⁻¹ between v=0 and v=6. Unreported T assumed 298 K.	EX	298	4.7(12)			2	
73 SCH/SCH1 k(v=7) = 1.58x10 ¹² cm ³ mol ⁻¹ s ⁻¹ . k decreases monotonically from v=0 to v=7.	EX	298	6.31(12)			2	
74 SCH/SCH v = 0.	EX	299-388	3.16(13)	0	503	2	
75 ALB/HOY v = 0.	EX	718-1111	(3.2±1.0)(13)	0	505±168	2	
CN + H₂ → HCN + H							
Cyanogen + Hydrogen molecule							
74 SCH/SCH	EX	298-388	6.31(13)	0	2667	2	
75 ALB/HOY	EX	718-1111	(6.0±2.0)(13)	0	2670±301	2	
77 SCH/WAG	EX	259-396	(6.0±2.0)(13)	0	2670±301	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CN(v=n) + NO(v'=0) → N ₂ + CO (a)							
→ CN(v=n-1) + NO(v'=1) (b)							
CN(v=n) + NO (+ M) → NOCN (+ M) (c)							
Cyanogen + Nitrogen oxide (NO)							
75 MUL/PHI k _a . n = 0.	ES	1500	7.3(12)				2
78 LAM/DUG ¹⁾ k _a . n = 0.	EX	300	(7.23±3.61)(10)				2
78 LAM/DUG ¹⁾ k _a + k _b . n = 1.	EX	300	(1.57±0.30)(11)				2
78 LAM/DUG ¹⁾ k _c . n = 0.	EX	300	(2.79±0.51)(17)				3
78 LAM/DUG ¹⁾ k _c . n = 1.	EX	300	(1.09±0.40)(17)				3
¹⁾ M = Ar. Flash-photolysis. Laser-induced fluorescence.							
CN + CO ₂ → CNO + CO							
Cyanogen + Carbon dioxide							
75 HAY/IVE	EX	1830-2400	(3.7±0.4)(12)	0	0		2
CN(v=n) + CH ₄ → HCN + CH ₃							
Cyanogen + Methane							
71 BUL/COO ¹⁾ n = 0. CN Absorption band: 0,0.	EX	300	(4.46±0.1)(13)				2
71 BUL/COO ¹⁾ n = 0. CN Absorption band: 4,4.	EX	300	(5.0±0.2)(11)				2
¹⁾ Radiolysis of C ₂ N ₂ + Ar.							
72 BUL/COO2 n = 0.	EX	300-377	1.29(13)	0	1006±96		2
74 SCH/SCH n = 0.	EX	298-388	3.16(13)	0	1459		2
77 SCH/WAG n = 0.	EX	259-396	(6.0±3.0)(12)	0	866±301		2
77 SCH/WAG n = 1.	EX	298	7.0(11)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CN + CD₄ → DCN + CD₃						
Cyanogen + Methane-d ₄						
72 BUL/COO2 CN(0,0) band.	EX	300	(2.4±0.4)(11)			2
72 BUL/COO2 CN(4,4) band.	EX	300	(3.5±0.2)(11)			2
CN + COS → SCN + CO						
Cyanogen + Carbon oxide sulfide						
79 ADD/LEI Time-resolved spectrophotometry. Lower-limit k.	EX	295	≥1.81(13)			2
CN(v=n) + CH=CH → products						
Cyanogen + Ethyne						
77 SCH/WAG v = 0.	EX	259-396	(3.0±1.0)(13)	0	0	2
77 SCH/WAG v = 1. Lower-limit k.	EX	298	≥1.5(14)			2
CN + CH₂=CH₂ → CH₂CH₂CN (a) → any other products (b)						
Cyanogen + Ethene						
71 BUL/COO ¹) CN Absorption band: 0,0.	EX	300	(1.16±0.15)(14)			2
71 BUL/COO ¹) CN Absorption band: 4,4.	EX	300	(1.35±0.20)(14)			2
¹) k _a . Radiolysis of C ₂ N ₂ + Ar.						
77 SCH/WAG ²) v = 0.	EX	259-396	(3.0±0.5)(13)	0	0	2
77 SCH/WAG ²) v=1.	EX	298	6.5(13)			2
²) k _{overall} .						
CN + CH₃CH₃ → HCN + CH₃CH₂						
Cyanogen + Ethane						
71 BUL/COO CN Absorption bands: 0,0 and 4,4. Radiolysis of C ₂ N ₂ + Ar.	EX	300	(1.45±0.10)(13)			2
72 BUL/COO2	EX	300-415	2.40(13)	0	192	2
72 BUL/COO2 B = 0 assumed.	EX	300-415	1.48(13)	0	0	2
74 SCH/SCH	EX	298	7.94(12)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CN + NCCN → [C₃N₃]						
Cyanogen + Ethanedinitrile						
72 BUL/COO1	EX	300-377	5.62(11)	0	1576	2
CN + CH₃CH=CH₂ → products						
Cyanogen + 1-Propene						
71 BUL/COO	EX	300	(1.6±0.2)(14)			2
CN Absorption band: 0,0. C ₂ N ₂ /Ar Radiolysis.						
CN + CH₃CH₂CH₃ → HCN + CH₃CH₂CH₂ (a) → HCN + (CH₃)₂CH (b)						
Cyanogen + Propane						
72 BUL/COO2	EX	300	(3.2±0.5)(13)			2
k _a + k _b .						
CN + CH₂=CHCH=CH₂ → products						
Cyanogen + 1,3-Butadiene						
71 BUL/COO	EX	300	(2.6±0.3)(14)			2
CN Absorption band: 0,0. C ₂ N ₂ /Ar Radiolysis.						
NCO + O₂ → NO + CO₂						
Cyanato + Oxygen molecule						
74 SCH/SCH	EX	298	7.94(11)			2
HCN (+ M) → H + CN (+ M)						
Hydrocyanic acid						
76 ROT/JUS	EX	2200-2700	5.72(16)	0	58940	2
M = Ar. Thermolysis behind shock-waves.						
80 ROT	EX	2200-2700	5.72(16)	0	59060	2
M = Ar. HCN Thermolysis behind shock-waves. Resonance-absorption. Same data given in 79 ROT/JUS1.						
82 SZE/HAN	EX	3570-5036	4.07(17)	0	44740±1060	2 1.29
M = Ar. HCN Thermolysis behind incident shock-waves in Ar. P = (128-218) torr.						
CH₃NH₂ (+ M) → CH₃ + NH₂ (+ M)						
Methanamine						
79 DOR/PCH ¹⁾	EX	1275-2400	6.92(10)	0	24233	1
Limiting high-pressure k.						
79 DOR/PCH ¹⁾	EX	1275-2400	3.16(13)	0	17685	2
Limiting low-pressure k.						
¹⁾ Reflected shock-waves. IR-emission techniques.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{N}=\text{N} \rightarrow \text{CH}_3 + \text{N}_2$ Diazenyl, methyl- 76 VID/WIL	EX	295	$\geq 3.0(6)$				1
$\text{CH}_3\text{NHNH}_2 \rightarrow \text{CH}_2=\text{NH} + \text{NH}_3$ (a) $\rightarrow \text{CH}_3\text{N}=\text{NH} + \text{H}_2$ (b) Hydrazine, methyl- 72 GOL/SOL	EX	943-1263	1.58(13)	0	27177		1
k_a . RRKM fit of experimental data.							
72 GOL/SOL	EX	943-1263	3.16(13)	0	28686		1
k_b . RRKM fit of experimental data.							
$\text{NH}_2\text{CO} (+ \text{M}) \rightarrow \text{NH}_2 + \text{CO} (+ \text{M})$ Amidogen, formyl- 73 YOK/BAC	RN	578	$(5.9 \pm 2.0)(12)$				1
M = HCONH ₂ . Limiting high-pressure k.							
73 YOK/BAC	RN	578	$(1.04 \pm 0.35)(17)$				2
k_o . M = HCONH ₂ . Low-pressure.							
$\text{NH}_2\text{CO} + \text{NH}_2\text{CO} \rightarrow \text{NH}_2\text{COCONH}_2$ (a) $\rightarrow \text{HNCO} + \text{HCONH}_2$ (b) Amidogen, formyl- 73 YOK/BAC	EX	578	$(3.1 \pm 1.0)(13)$				2
$k_a + k_b$.							
$\text{CH}_3\text{NO}^\dagger \rightarrow \text{CH}_3 + \text{NO}$ Methane, nitroso- 74 TIT/BAL	ES	443	2.0(7)				1
$\text{CH}_3\text{NO}^\dagger$ generated by reacting CH_3 with NO.							
$\text{CH}_3\text{ONO} (+ \text{M}) \rightarrow \text{HCHO} + \text{HNO} (+ \text{M})$ (a) $\rightarrow \text{CH}_3\text{O} \cdot + \text{NO} (+ \text{M})$ (b) Nitrous acid methyl ester 75 BAT/MCC	ES	393-473	1.0(10)	0	16004		1
k_a .							
77 BAT/MIL3	ES	440-473	3.98(13)	0	19376±503		1 3.98
k_a .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 BAT/MIL k_b .	ES	393-473	6.31(15)	0	20735±503	1	2.51
75 BAT/MCC k_b .	ES	393-473	6.31(15)	0	20735±503	1	2.51
77 BAT/MIL3 k_b .	ES	440-473	6.31(15)	0	20745±503	1	3.98
75 MAL/GAN M = Ar. Incident and reflected shockwaves. P = (0.8-5) atm.	EX	715-1118	2.29(16)	0	15299±428	2	1.66
 $\text{CH}_3\text{NO}_2 (+ \text{M}) \rightarrow \text{CH}_3 + \text{NO}_2 (+ \text{M})$ Methane, nitro-							
72 GLA/TRO M = Ar. Limiting high-pressure k.	EX	900-1400	1.78(16)	0	29441±252	1	
72 GLA/TRO M = Ar. Low-pressure k.	EX	900-1370	1.26(17)	0	21137	2	
 $\text{CH}_3\text{ONO}_2 \rightarrow \text{CH}_3\text{O} + \text{NO}_2$ Nitric acid methyl ester							
77 BAT/MIL3	ES	440-473	5.01(15)	0	20382±503	1	3.98
 $\text{CH}_3\text{O}_2\text{NO}_2 (+ \text{M}) \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2 (+ \text{M})$ Peroxynitric acid methyl ester							
82 BAH/SIM ¹⁾ Experimental k. P ~ 350 torr.	EX	256-268	6.0(15)	0	10619±755	1	
82 BAH/SIM ¹⁾ Optimization based on combination of the above experimental data with k_{-1} and thermodynamic data.	DE	256-268	(6.0±3.0)(15)	0	10720±151	1	
82 BAH/SIM ¹⁾ Limiting high-pressure k.	CO	256-268	2.1(16)	0	10921±151	1	
82 BAH/SIM ¹⁾ Limiting low-pressure k. Both limiting k values are evaluations based on the P-dependence of k_{-1} .	DE	256-268	2.0(20)	0	10141±151	2	
¹⁾ $\text{CH}_3\text{O}_2\text{NO}_2$ decomposition in a Pyrex reaction cell with vacuum system. UV-spectrometry. $\text{CH}_3\text{O}_2\text{NO}_2$ generated by $\text{Cl}_2/\text{O}_2/\text{CH}_4/\text{NO}_2$ photolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err.	units factor
$C_2(X^1\Sigma_g^+ = A^3\Pi_g) (+ M) \rightarrow C + C (+ M)$							
Carbon dimer							
75 BEC/MAC M = Ar. Shock-wave pyrolysis of CH=CH in Ar.	EX	4860-6920	3.71(14)	0	69885±7097	2	1.86
$C_2(X^1\Sigma_g^+) + O_2 \rightarrow CO^* + CO$ (a) → any other products (b)							
Carbon dimer + Oxygen molecule							
80 REI/MAN1 k_a . $CH_2=CHCN/O_2$ Multiphoton dissociation. CO^* is in an electronically excited triplet state.	EX	300	(1.81±0.12)(12)			2	
79 PAS/MCD $k_{overall}$. $CF_3C\equiv CF_3$ Multiphoton laser photo-dissociation. Laser-induced fluorescence.	EX	298	(1.70±0.05)(12)			2	
80 MAN/REI $k_{overall}$. $CH_2=CN$ or $CHCl=CCl_2$ Multiphoton laser dissociation in a fluorescence chamber.	CO	298	1.63(12)			2	
82 PIT/PAS ¹⁾ $C_2(X^1\Sigma_g^+)$ reacts as fast as $C_2(a^3\Pi_u)$.	EX	300-600	(6.44±1.51)(12)	0	337±81	2	
82 PIT/PAS ¹⁾ $C_2(X^1\Sigma_g^+)$ reacts much faster than $C_2(a^3\Pi_u)$.	EX	300-600	(2.00±0.60)(13)	0	604±101	2	
¹⁾ $k_{overall}$. Dye-laser induced fluorescence. C_2 produced by multiphoton UV-photolysis of $CF_3=CCF_3$.							
$C_2(a^3\Pi_u) + O_2 \rightarrow CO(A^1\Pi) + CO$ (a) → $CO^* + CO$ (b)							
Carbon dimer + Oxygen molecule							
79 FIL/HAN k_a . Laser-induced fluorescence.	EX	298	2.05(12)			2	
80 REI/MAN1 k_b . $CH_2=CHCN/O_2$ Multiphoton dissociation. CO^* is an electronically excited triplet.	EX	300	(1.81±0.12)(12)			2	
79 DON/PAS $k_{overall}$. CH=CH Multiphoton photolysis. Dye-laser induced fluorescence. P(N ₂) = (10-45) torr.	EX	298	(1.78±0.04)(12)			2	
80 MAN/REI $k_{overall}$. $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation in a fluorescence chamber.	CO	298	1.63(12)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 PIT/PAS k_{overall} . $C_2(a^3\Pi_u)$ is assumed to react as fast as $C_2(X^1\Sigma_g^+)$. Dye-laser induced fluorescence. C_2 produced by Multiphoton Photolysis of $CF_3=CCF_3$.	EX	300-600	(6.44±1.51)(12)	0	337±81	2
$C_2(X^1\Sigma_g^+) + H_2O \rightarrow$ products Carbon dimer + Water						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(a^3\Pi_u) + H_2O \rightarrow$ products Carbon dimer + Water						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(X^1\Sigma_g^+) + N_2 \rightarrow$ products Carbon dimer + Nitrogen molecule						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(a^3\Pi_u) + N_2 \rightarrow$ products Carbon dimer + Nitrogen molecule						
80 REI/MAN2 $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
$C_2(X^1\Sigma_g^+) + NO \rightarrow CN(X^2\Sigma^+) + CO$ (a) $\rightarrow CN(A^2\Pi) + CO$ (b) Carbon dimer + Nitrogen oxide (NO)						
82 LE k_a . Premixed fuel-rich $CH=CH/NO$ flames, at 250-600 nm. P = 80 torr.	ES	2700	3.6(14)			2
80 REI/MAN2 $k_a + k_b$. $CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	1.26(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$C_2(a^3\Pi_u) + NO \rightarrow CN(X^2\Sigma^+) + CO$ (a)						
$\rightarrow CN(B^2\Sigma^+) + CO$ (b)						
$\rightarrow CN(A^2\Pi) + CO$ (c)						
$\rightarrow CN(X^2\Sigma^+) + CO(a^3\Pi)$ (d)						
Carbon dimer + Nitrogen oxide (NO)						
79 REI/MAN ¹⁾	EX	298	(4.40±0.54)(13)			2
k determined by using LIF to monitor $C_2(a^3\Pi_u)$.						
79 REI/MAN ¹⁾	EX	298	(4.52±0.18)(13)			2
k determined from $CN(B^2\Sigma^+ \rightarrow X^2\Sigma^+)$ chemiluminescence.						
79 REI/MAN ¹⁾	EX	298	(4.40±0.18)(13)			2
k determined from $CN(A^2\Pi \rightarrow X^2\Sigma^+)$ chemiluminescence.						
¹⁾ $k_a + k_b + k_c + k_d$.						
Ethylene, or Vinyl cyanide Multiple-photon dissociation.						
Time-resolved Chemiluminescence.						
Laser-induced Fluorescence.						
$P(CH_2=CHCN) = (1-10)$ mtorr.						
$P(CH_2=CH_2) = (1-10)$ mtorr.						
$P(Ar) = (50-500)$ mtorr.						
$C_2(X^1\Sigma_g^+) + CO_2 \rightarrow$ products						
Carbon dimer + Carbon dioxide						
80 REI/MANZ	EX	300	<1.81(10)			2
$CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation.						
Laser-induced fluorescence.						
Upper-limit k.						
$C_2(a^3\Pi_u) + CO_2 \rightarrow$ products						
Carbon dimer + Carbon dioxide						
80 REI/MANZ	EX	300	<1.81(10)			2
$CH_2=CHCN$ or $CHCl=CCl_2$ Multiphoton dissociation.						
Laser-induced fluorescence.						
Upper-limit k.						
$C_2(X^1\Sigma_g^+) + CH_4 \rightarrow CH=C + CH_3$ (a)						
$\rightarrow CH_3C=CH$ (b)						
Carbon dimer + Methane						
79 PAS/MCD	EX	298	(1.13±0.03)(13)			2
k_a .						
$CF_3C=CF_3$ Multiphoton laser photodissociation.						
Laser-induced fluorescence.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 FIT/PAS k _D . Dye-laser induced fluorescence. C ₂ produced by multiphoton UV-Photolysis of CF ₃ C=CCF ₃ .	EX	300-600	(3.04±0.09)(13)	0	297±10	2
80 REI/MAN2 k _{overall} . CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(1.02±0.12)(13)			2
C₂(a³Π_u) + CH₄ → products						
Carbon dimer + Methane						
79 DON/PAS CH=CH Multiphoton photolysis. Dye-laser induced fluorescence. Upper-limit k. P(CH ₄) = (0-250) torr. P(N ₂) = (0-10) torr.	EX	298	<6.02(7)			2
80 PAS/BAR CF ₃ C=CCF ₃ Multiphoton UV-photolysis. Dye-laser induced fluorescence. P(CF ₃ C=CCF ₃) = (1.5-4.0) mtorr. P(CH ₄) ~ (10-170) torr.	EX	337-605	(9.94±1.20)(12)	0	2805±55	2
80 REI/MAN2 CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.	EX	300	<1.81(10)			2
C₂(X¹Σ_g⁺) + CH=CH → products						
Carbon dimer + Ethyne						
80 REI/MAN2 CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(2.59±0.24)(14)			2
C₂(a³Π_u) + CH=CH → products						
Carbon dimer + Ethyne						
79 DON/PAS CH=CH Multiphoton photolysi Dye-laser induced fluorescence. P-independent.	EX	298	(5.78±0.18)(13)			2
C₂(X¹Σ_g⁺) + CH₂=CH₂ → products						
Carbon dimer + Ethene						
79 PAS/MCD CF ₃ C=CCF ₃ Multiphoton laser photodissociation. Laser-induced fluorescence.	EX	298	(1.96±0.03)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$C_2(a^3\Pi_u) + CH_2=CH_2 \rightarrow$ products						
Carbon dimer + Ethene						
79 DON/PAS CH=CH Multiphoton photolysis. Dye-laser induced fluorescence. P(N ₂) = (10-60) torr.	EX	298	(8.67±0.36)(13)			2
81 PAS/PIT CF ₃ C=CCF ₃ or C ₆ H ₆ Multiphoton laser dissociation. Laser-induced fluorescence.	EX	300-600	(7.23±0.96)(13)	0	-5±46	2
$C_2(X^1\Sigma_g^+) + CH_3CH_3 \rightarrow CH=C + CH_3CH_2$						
Carbon dimer + Ethane						
79 PAS/MCD CF ₃ C=CCF ₃ Multiphoton laser photodissociation. Laser-induced fluorescence.	EX	298	(9.58±0.30)(13)			2
$C_2(a^3\Pi_u) + CH_3CH_3 \rightarrow CH=C + CH_3CH_2$						
Carbon dimer + Ethane						
79 DON/PAS CH=CH Multiphoton photolysis. Dye-laser induced fluorescence. P(N ₂) = (10-60) torr.	EX	298	(7.83±0.36)(11)			2
81 PAS/PIT CF ₃ C=CCF ₃ or C ₆ H ₆ Multiphoton laser dissociation. Laser-induced fluorescence.	EX	300-600	(1.46±0.06)(13)	0	919±15	2
$C_2(X^1\Sigma_g^+) + CH_2=CHCN \rightarrow$ products						
Carbon dimer + 2-Propenenitrile (Acrylonitrile)						
80 REI/MAN2 CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(2.65±0.18)(14)			2
$C_2(a^3\Pi_u) + CH_2=CHCN \rightarrow$ products						
Carbon dimer + 2-Propenenitrile (Acrylonitrile)						
80 REI/MAN2 CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(3.43±0.24)(13)			2
$C_2(X^1\Sigma_g^+) + CH_2=C=CH_2 \rightarrow$ products						
Carbon dimer + 1,2-Propadiene						
80 REI/MAN2 CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.	EX	300	(2.83±0.24)(14)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$C_2(a^3\Pi_u) + CH_2=C=CH_2 \rightarrow$ products						
Carbon dimer + 1,2-Propadiene						
80 REI/MAN2	EX	300	(1.57±0.12)(14)			2
CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.						
$C_2(X^1\Sigma_g^+) + CH_3CH_2CH_3 \rightarrow$ products						
Carbon dimer + Propane						
80 REI/MAN2	EX	300	(1.99±0.12)(14)			2
CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence. Upper-limit k.						
$C_2(a^3\Pi_u) + CH_3CH_2CH_3 \rightarrow$ CH=C + CH₃CH₂CH₂ (a) → CH=C + (CH₃)₂CH (b)						
Carbon dimer + Propane						
81 PAS/PIT	EX	300-600	(1.11±0.10)(13)	0	97±36	2
k _a + k _b . CF ₃ C≡CCF ₃ Multiphoton laser dissociation. Laser-induced fluorescence.						
80 REI/MAN2	EX	300	(1.00±0.06)(14)			2
k _{overall} . CH ₂ =CHCN or CHCl=CCl ₂ Multiphoton dissociation. Laser-induced fluorescence.						
$C_2(a^3\Pi_u) + CH_3CH_2CH_2CH_3 \rightarrow$ CH=C + CH₃CH₂CH₂CH₂ (a) → CH=C + CH₃CH₂CHCH₃ (b)						
Carbon dimer + Butane						
81 PAS/PIT	EX	300-600	(2.95±0.30)(13)	0	71±41	2
CF ₃ C≡CCF ₃ or C ₆ H ₆ Multiphoton laser dissociation. Laser-induced fluorescence.						
$C_2O + CH\equiv CH \rightarrow$ products						
Carbon oxide (C ₂ O) + Ethyne						
80 DON/PIT	EX	298	<6.02(9)			2
C ₃ O ₂ photodissociation at 266 nm. Dye-laser induced fluorescence. Upper-limit k.						
$C_2O + CH_2=CH_2 \rightarrow$ products						
Carbon oxide (C ₂ O) + Ethene						
80 DON/PIT	EX	298	<6.02(9)			2
C ₃ O ₂ photodissociation at 266 nm. Dye-laser induced fluorescence. Upper-limit k.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C₂O + (CH₃)₂C=CH₂ → products						
Carbon oxide (C ₂ O) + 1-Propene, 2-methyl-						
80 DON/PIT	EX	298	(6.75±0.30)(10)			2
C ₃ O ₂ Laser photodissociation at 266 nm. Dye-laser induced fluorescence.						
CH≡C (+ M) → C₂ + H (+ M)						
Ethynyl						
75 BEC/MAC ¹⁾	DE	4860-6920	3.61(15)	0	71930	2
M = Ar.						
75 BEC/MAC ¹⁾	DE	4860-6920	6.02(13)	0	14554	2
M = H.						
¹⁾ Shock-wave pyrolysis. CH≡CH in Ar. Best-fit.						
CH≡C + O₂ → products						
Ethynyl + Oxygen molecule						
75 LAN/WAG	EX	320	≈3.3(12)			2
Discharge-flow. Mass-spectrometry. P = 4.1 torr.						
82 REN/SHO	EX	300	(1.26±0.18)(13)			2
M = He or Ar. Vacuum chamber. CH≡C produced by Laser-Photolysis of CH≡CH, CH≡CBr, CH≡CHO, or CH≡CCF ₃ in presence of O ₂ , at 192 nm. Time-resolved chemiluminescence. IR-Spectro- scopy. P(Ar, or He) = (210-860) mtorr. P(CH≡CH) = (5-25) mtorr. P(O ₂) = (80-500) mtorr.						
CH≡C + H₂ → CH≡CH + H						
Ethynyl + Hydrogen molecule						
74 YAM/LAV	DE	1063-1233	6.02(12)	0	3271	2
k ₁ = k ₋₁ K.						
75 LAN/WAG	EX	320	≈1.0(11)			2
Discharge-flow. Mass-spectrometry. P = 4.2 torr.						
79 LAU/BAS	EX	298	4.9(-3)			2
Vacuum-UV flash-photolysis. Kinetic-spectroscopy. Gas-chromatography.						
k _{ref} : CH≡CH + CH≡C → H + CH≡CC=CH						
80 TAN/GAR2	ES	625-3400	3.39(13)	0	0	2
CH≡CH Pyrolysis. Based on a modelling study.						
81 KOI/MOR1	ES	1800-2600	2.51(12)	0	0	2
CH≡CH Pyrolysis behind incident shock-waves. P = 380 torr. Based on a modelling study.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 OKA CH=CH/H ₂ photolysis at 147 nm. P(CH=CH) = (0.1-10) torr.	EX	298	(7.75±0.68)(-3)			2
81 REN/SHO CH=C produced by laser photolysis of CH=CH, CH=CBr, or CH=CCHO in presence of O ₂ , at 193 nm. Time-Resolved Chemiluminescence. P(Ar, or He) = (180-400) mtorr. P(O ₂) = (20-400) mtorr.	EX	300	(7.23±1.81)(12)			2
CH=C + CH₄ → CH=CH + CH₃						
Ethyne + Methane						
73 CUL/HUC ¹⁾	RL	298	(1.6±0.5)(-2)			2/2
73 CUL/HUC ¹⁾	RL	478	1.1(-1)			2/2
73 CUL/HUC ¹⁾	RL	298-478	(2.36±1.09)	0	1508±153	2/2
Calculated from the reported reverse ratio.						
¹⁾ k _{ref} : CH=C + CH=CBr → CH=CC=CH + Br						
81 LAU Flash-photolysis. Kinetic-spectroscopy. k independent of He over the (20-700) torr. P-range.	EX	297	(7.23±1.20)(11)			2
81 OKA Photolysis of CH=CH/CH ₄ mixtures at 147 nm. P(CH=CH) = (0.1-10) torr. k _{ref} : CH=CH + CH=H → CH=CC=CH + H	RL	298	(3.20±0.18)(-2)			2/2
81 REN/SHO CH=C produced by laser photolysis of CH=CH, CH=CBr, or CH=CCHO in presence of O ₂ , at 193 nm. Time-resolved Chemiluminescence. P(Ar, He) = (180-400) mtorr. P(O ₂) = (20-400) mtorr.	EX	300	(2.89±0.60)(12)			2
CH=C + CH=CH → CH=CC=CH + H						
Ethyne + Ethyne						
73 CUL/HUC	ES	298	1.0(11)	0	1504	2
75 LAN/WAG Discharge-flow. Mass-spectrometry. P = 4.1 torr.	EX	320	≈3.0(13)			2
79 LAU/BAS Vacuum-UV flash-photolysis. Kinetic Spectroscopy.	EX	298	(1.87±0.12)(13)			2
80 FRA/JUS Pyrolysis of CH=CH and CH=CC=CH in Ar, behind shock-waves. Data-fit based on a proposed mechanism. Total Conc. = (0.4-1.6)×10 ¹⁹ molec.cm ⁻³ .	ES	2300-2700	(3.5±0.5)(13)	0	0	2

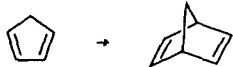
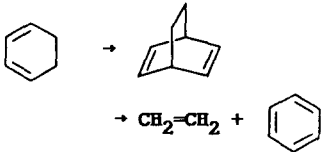
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k/ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH≡C + CD≡CD → CH≡CC=CD + D						
Ethyne + Ethyne-d ₂						
73 CUL/HUC k _{ref} : CH≡C + CD≡CD → CH≡CD + CD≡C	RL	298	(2.8±2.5)			2/2
73 CUL/HUC Calculated from the reported reverse ratio. k _{ref} : CH≡C + CH≡CBr → CH≡CC=CH + Br	RL	298	(6.7±1.6)(-1)			2/2
CH≡C + CH₃CH₃ → CH=CH + CH₃CH₂						
Ethyne + Ethane						
73 CUL/HUC k _{ref} : CH≡C + CH≡CBr → CH≡CC=CH + Br	RL	298	(5.4±0.4)(-1)			2/2
81 LAU Flash-photolysis. Kinetic-spectroscopy. k independent of He over the (20-700) torr. P-range.	EX	297	(3.91±0.24)(12)			2
CH≡C + CD₃CD₃ → CH=CD + CD₃CD₂						
Ethyne + Ethane-d ₆						
81 LAU Flash-photolysis. Kinetic-spectroscopy. k independent of He over the (20-700) torr. P-range.	EX	297	(1.87±0.30)(12)			2
CH≡C + CH₃C≡CH → CH=CH + CH₂C≡CH (a) → CH≡CC=CH + CH ₃ (b) → CH≡CC=CCH ₃ + H (c)						
Ethyne + 1-Propyne						
73 CUL/HUC k _a /k _c .	RL	298	(2.5±0.3)(1)			2/2
73 CUL/HUC k _b /k _c .	RL	298	(9.9±1.0)			2/2
73 CUL/HUC ¹⁾ k _{ref} : CH≡C + CH≡CBr → CH≡CC=CH + C≡CBr	RL	298	(4.43±0.58)(-2)			2/2
73 CUL/HUC ¹⁾ k _{ref} : CH≡C + CH≡CBr → CH≡CC=CH + Br	RL	298	(2.38±0.95)(-1)			2/2
¹⁾ k _c /k _{ref} . Calculated from the reverse ratio.						
CH≡C + CH≡CC=CH → CH=CH + CH≡CC=C (a) → CH≡CC=CC=CH + H (b)						
Ethyne + 1,3-Butadiene						
73 CUL/HUC k _a /k _b .	RL	298	(1.1±0.2)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 CUL/HUC k_b/k_{ref} . Calculated from the reverse ratio. k_{ref} : $CH\equiv C + CH\equiv CBr \rightarrow CH=CH + C\equiv CBr$	RL	298	(1.71±0.29)				2/2
80 FRA/JUS k_b . $CH=CH$ and $CH=CC=CH$ Pyrolysis in Ar behind shock-waves. Data-fit on the basis of a given mechanism. Total Conc. = $(0.4-1.6)\times 10^{19}$ molec.cm ⁻³ .	ES	2400-2700	(2.5±1.5)(13)	0	0		2
$CH\equiv C + CH_2=C=CH \rightarrow CH=CH + CH=C=CH$ Ethyne + 1-Buten-3-yne							
80 TAN/GAR2 $CH=CH$ Pyrolysis. Based on modelling study.	ES	625-3400	3.98(13)	0	0		2
$CH\equiv C + (CH_3)_4C \rightarrow CH=CH + (CH_3)_3CCH_2$ Ethyne + Propane, 2,2-dimethyl-							
73 CUL/HUC k_{ref} : $CH\equiv C + CH\equiv CBr \rightarrow CH=CC=CH + Br$	RL	298	(9.1±0.4)(-1)				2/2
$CH=CH (+ M) \rightarrow CH\equiv C + H (+ M)$ (a) $\rightarrow C + C + H_2 (+ M)$ (b)							
Ethyne							
74 ALT k_a .	EX	1700-2000	1.0(15)	0	55360		1
78 CUN/FUS $k_{overall}$. M = Ar. Incident shock-waves. P = (1-2) bar.	ES	1500-2000	1.58(7)	0	24899		1
75 BEC/MAC ¹⁾ k_a . M = Ar.	DE	4860-6920	6.02(15)	0	75419		2
75 BEC/MAC ¹⁾ k_a . M = H.	DE	4860-6920	5.42(13)	0	12028		2
¹⁾ $CH=CH$ Shock-wave pyrolysis in Ar. Best-fit of experimental data.							
80 FRA/JUS k_a . M = Ar. $CH=CH$ and $CH=CC=CH$ pyrolysis in Ar, behind shock-waves. Total Conc. = $(0.4-1.6)\times 10^{19}$ molec.cm ⁻³ .	EX	2100-3000	(3.6±0.6)(16)	0	53600±400		2
82 THR/WIN k_b . M = Ar. $CH=CH$ decomposition in an Ar plasma. Mass-spectrometry.	EX	3900-4250	1.00(14)	0	30673±8420		2 10.0

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}=\text{CH} + \text{CH}=\text{CH} \rightarrow \text{CH}=\text{CCH}=\text{CH} + \text{H}$ (a) $\rightarrow \text{CH}=\text{CC}=\text{CH} + \text{H} + \text{H}$ (b) $\rightarrow \text{CH}_2=\text{CCH}=\text{CH}$ (c)							
Ethyne							
80 TAN/GAR2 k_a . $\text{CH}=\text{CH}$ pyrolysis. Modelling study.	ES	625-3400	2.00(12)	0	23095	2	
80 BAR/DOV 1) k_a .	EX	2650	1.98(10)			2	
80 BAR/DOV 1) k_a . Based on present and previous k 's.	SE	1600-2650	6.0(13)	0	20634	2	
1) $\text{CH}=\text{CH}$ pyrolysis behind shock-waves.							
80 FRA/JUS 2) k_a .	ES	1845-2000	(1.51±0.79)(8)	0	0	2	
80 FRA/JUS 2) k_b .	ES	1845-2000	(3.0±1.0)(8)	0	0	2	
2) $\text{CH}=\text{CH}/\text{CH}=\text{CC}=\text{CH}$ Pyrolysis in Ar behind shock-waves. Data-fit based on a proposed mechanism. Total Conc. = (0.4-1.6)×10 ¹⁹ molec.cm ⁻³ .							
77 OGU1 3)	EX	1000-1670	2.45(14)	0	23352±705	2	1.82
77 OGU2 3)	EX	1000-1600	(1.48±0.18)(14)	0	22245±755	2	
3) k_c .							
$\text{CH}=\text{CH} + $ 							
Ethyne + 1,3-Cyclopentadiene							
→ Bicyclo[2.2.1]hepta-2,5-diene (2,5-Norbornadiene)							
75 WAL/WEL	EX	525-756	3.24(7)	0	12174±75	2	1.12
Static system. Gas-chromatography. Diels-Alder addition of $\text{CH}=\text{CH}$ to 1,3-Cyclopentadiene.							
$\text{CH}=\text{CH} + $ 							
Ethyne + 1,3-Cyclohexadiene							
→ Bicyclo[2.2.2]octa-2,5-diene → Ethene + Benzene							
82 HUY/LEE	EX	450-592	3.09(10)	0	13664±60	2	1.12
Thermal Diels-Alder addition of $\text{CH}=\text{CH}$ to 1,3-Cyclohexadiene. NMR-Spectrometry. Gas-chromatography. Static system. P(1,3-Cyclohexadiene) = (8-62) torr. P($\text{CH}=\text{CH}$) = (25-112) torr.							






4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₂=CH (+ M) → CH=CH + H (+ M)						
Ethenyl						
73 PEE/MAH2	ES	1500	2.0(12)			2
CH₂=CH + CH≡CH → CH₂-CHC≡CH + H						
Ethenyl + Ethyne						
80 TAN/GAR2	ES	625-3400	1.58(13)	0	12630	2
CH≡CH Pyrolysis. Based on a modelling study.						
CH₂=CH + CH₂=CH → CH=CH + CH₂=CH₂ (a)						
→ CH₂=CHCH=CH₂ (b)						
Ethenyl						
75 IBU/TAK	RL	296	8.7(-2)			2/2
k _a /k _b . Conventional vacuum system.						
CH₂=CH + CH₃CH₂ → CH=CH + CH₃CH₃ (a)						
→ CH₂=CH₂ + CH₂=CH₂ (b)						
→ CH₃CH₂CH=CH₂ (c)						
Ethenyl + Ethyl						
75 IBU/TAK ¹⁾	RL	296	3.69(-1)			2/2
k _a /k _c .						
75 IBU/TAK ¹⁾	RL	296	6.8(-1)			2/2
k _b /k _c .						
¹⁾ Conventional vacuum system.						
CH₂=CH₂ (+ M) → CH₂=CH + H (+ M) (a)						
→ CH=CH + H₂ (+ M) (b)						
Ethene						
73 ROT/JUS ¹⁾	EX	1675-2210	1.78(17)	0	39004	2
77 JUS/ROT ¹⁾	EX	1700-2200	(3.8±1.3)(17)	0	49400±900	2
80 TAN/GAR1 ¹⁾	EX	2000-2450	3.09(17)	0	48114	2
Pyrolysis behind incident shock-waves.						
Total Conc. = (1.1-2.2)×10 ¹⁸ molec. ⁻³ .						
¹⁾ k _a . M = Ar.						




4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2=\text{CH} + \text{CH}_3\text{CH}_2$ (a)							
$\rightarrow \square$ (b)							
Ethene							
81 AYR/BAC k_a . Static system pyrolysis. Gas-chromatography. k determined relative to the reaction: $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_2\text{CH}=\text{CH}_2$	RN	750	1.58(16)	0	33719	2	
72 QUI/KNE k_b .	EX	723-786	6.92(10)	0	22043	2	1.15
$\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$							
Ethene + 1-Propene							
78 RIC/BAC Static system pyrolysis. P(olefin) = (33-300) torr.	EX	682-754	2.82(10)	0	18621±503	2	2.0
$\text{CH}_2=\text{CH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ (a)							
$\rightarrow \text{cis-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ (b)							
Ethene + 2-Butene, (Z)-							
78 RIC/SCA k_a . Static system pyrolysis. P(olefin) = (20-200) torr.	EX	689-754	1.12(10)	0	18369±503	2	2.0
77 SCA/BAC k_b . A-factor recalculated from the reported experimental data. Average k.	EX	663-703	(1.28±0.16)(12)	0	24270±71	2	
77 SCA/RIC k_b . Determined from present and literature data for the rate of geometric isomerization of 1,2- Dimethyl-cyclobutane. Static system. P = 12 atm.	RN	693	8.0(-4)			2	
$\text{CH}_2=\text{CH}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$							
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2$ (a)							
$\rightarrow \text{trans-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ (b)							
Ethene + 2-Butene, (E)-							
78 RIC/SCA k_a . Static system pyrolysis. P(olefin) = (20-200) torr.	EX	689-754	3.55(10)	0	18621±503	2	2.0
77 SCA/BAC k_b . A-factor recalculated from the reported experimental data.	EX	663-703	(4.49±0.89)(11)	0	23136±120	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 SCA/BAC k_b/k_{ref} . Average, estimated ratio. k_{ref} : $CH_2=CH_2 + cis-CH_3CH=CHCH_3$ $\rightarrow cis-CH_3CHCH(CH_3)CH_2CH_2$	RL	663-703	(1.80±0.10)	0	0	2/2	
77 SCA/RIC ¹⁾ k_b/k_{ref} . k_{ref} : $CH_2=CH_2 + cis-CH_3CH=CHCH_3$ $\rightarrow cis-CH(CH_3)CH(CH_3)CH_2CH_2$	RL	693	(1.86±0.1)			2/2	
77 SCA/RIC ¹⁾ k_b . Determined from present and literature data for the rate of geometric isomerization of 1,2-Dimethyl-cyclobutane. ¹⁾ Static system. P = 12 atm.	RN	693	1.48(-3)			2	
$CH_2=CH_2 + (CH_3)_2C=CH_2 \rightarrow CH_3CH_2C(CH_3)=CH_2$ Ethene + 1-Propene, 2-methyl-							
78 RIC/BAC Pyrolysis in a static system. P(olefin) = (33-300) torr.	EX	682-754	1.78(11)	0	19124±503	2	2.0
$CH_2=CH_2 + $  $\rightarrow $ 							
Ethene + 1,3-Cyclopentadiene \rightarrow Bicyclo(2.2.1)hept-2-ene (Norbornene)							
76 WAL/WEL Diels-Alder addition of Ethene to 1,3-Cyclopentadiene in a static system. Gas-chromatography.	EX	521-570	3.89(10)	0	11912±785	2	4.27
$CH_2=CH_2 + CH_2=C(CH_3)CH=CH_2 \rightarrow $ 							
Ethene + 1,3-Butadiene, 2-methyl- \rightarrow Cyclohexene, 1-methyl-							
78 SIM Single-pulse shock-tube. From k_r and thermodynamic data.	DE	1000-1180	1.32(11)	0	14900	1	
$CH_2=CH_2 + $  $\rightarrow CH_3CH_3 + $ 							
Ethene + Cyclopentene \rightarrow Ethane + 1,3-Cyclopentadiene							
80 LAL/BAC Static system. P(Total) = (150-350) torr.	EX	598-778	1.0(15)	0	25013	2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CH}_2 + $  $ \rightarrow $ 						
Ethene + 1,3-Cyclohexadiene \rightarrow Bicyclo[2.2.2]oct-2-ene						
80 HUY/RIG Vacuum system. Gas-chromatography. Diels-Alder addition of Ethene to 1,3-Cyclohexadiene.	EX	466-591	4.57(9)	0	13070 \pm 25	2 1.05
77 TAN k_p . M = Ar. Pyrolysis in shock-waves. Laser-schlieren. P = (0.9-1.7) kPa. of Ethene in Ar.	EX	2000-2500	1.2(17)	0	38700	2
77 JUS/ROT k_p . M = Ar.	EX	1700-2200	(2.6 \pm 0.5)(17)	0	39900 \pm 500	2
80 TAN/GAR1 k_p . M = Ar. Ethene pyrolysis. Incident shock-waves. Total Conc. = (1.1-2.2) $\times 10^{18}$ molec.cm ⁻³ .	EX	2000-2450	2.95(17)	0	40897	2
78 CUN/FUS k_{overall} . M = Ar. Incident shock-waves. P = (1-2) bar.	ES	1500-2000	6.31(6)	0	27305	1
$\text{CH}_3\text{CH}_2 (+ \text{M}) \rightarrow \text{CH}_2=\text{CH}_2 + \text{H} (+ \text{M})$						
Ethyl						
79 PRA/ROG1 M = Ar. Ethane pyrolysis in a wall-less reactor. P(Ar) = 600 torr. Gas-chromatography. Data-fit.	CO	941-1073	3.16(13)	0	21050 \pm 1443	1 5.01
81 COR/MAR Ethane pyrolysis. Flow-reactor. Based on a proposed mechanism. P = 40 torr.	ES	803	2.0(2)			1
76 CHE/BAC	CO	995	3.29(4)			2
80 PAC/WIM2 Estimated k. Ethane pyrolysis. Flow-reactor. Gas-chromatography. P = 100 torr.	RN	903	(3.6 \pm 0.5)(3)			2
$\text{CH}_3\text{CH}_2 + \text{O}_2 \rightarrow \text{CH}_2=\text{CH}_2 + \text{HO}_2$ (a)						
$\quad \quad \quad \rightarrow \text{CH}_3\text{CH}_2\text{O}_2$ (b)						
$\quad \quad \quad \rightarrow \text{CH}_3\text{CHO} + \text{OH}$ (c)						
$\quad \quad \quad \rightarrow $  $ + \text{OH}$ (d)						
Ethyl + Oxygen molecule						
71 BAL/LAN k_a/k_{ref} . Estimated ratio. k_{ref} : $\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CHO} \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CO}$	RL	713	(4.1 \pm 0.5)(1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
71 BAK/BAL ¹⁾	ES	896	1.0(11)			2
71 BAL/LAN ¹⁾	ES	713	8.2(10)			2
80 BAL/PIC ¹⁾ Static system. Gas-chromatography.	EX	673-813	8.51(11)	0	1949	2
81 PLU/RVA2 ¹⁾ ²⁾ M = He. k is independent of [He].	EX	295	(1.26±0.30)(11)			2
¹⁾ k _a						
81 PLU/RVA2 ²⁾ k _b . M = He. k strongly dependent on [He]. Limiting high-pressure k.	ES	295	~2.65(12)			2
71 BAK/BAL k _c .	ES	773	3.4(8)			2
71 BAK/BAL k _d .	ES	773	2.6(9)			2
81 PLU/RVA2 ²⁾ k _{overall} . M = He. [He] = 2.0x10 ¹⁶ molec.cm ⁻³ . k increases with [He].	EX	295	(7.23±1.80)(11)			2
81 PLU/RVA2 ²⁾ k _{overall} . M = He. [He] = 3.4x10 ¹⁷ molec.cm ⁻³ . k increases with [He].	EX	295	(2.17±0.54)(12)			2
²⁾ Flow-reactor. Mass-spectrometry. CH ₃ CH ₂ produced by reaction of Cl with Ethane.						
CH₃CH₂ + O₃ → products						
Ethyl + Ozone						
82 PAL Photoionization Mass-spectrometry. CH ₃ CH ₂ generated by photodissociation of CH ₃ CH ₂ NO ₂ . P = 2 torr.	EX	298	(1.40±0.22)(13)			2
CH₃CH₂ + H₂ → CH₃CH₃ + H						
Ethyl + Hydrogen molecule						
71 BAL/LAN k _{ref} : CH ₃ CH ₂ + CH ₃ CH ₂ CHO → CH ₃ CH ₃ CH ₂ CO Estimated ratio.	RL	713	(1.24±0.17)(-1)			2/2
71 BAL/LAN	ES	713	2.15(8)			2
82 CAO/BAC Cylindrical quartz reactor, with packed or unpacked vessels. Static system. CH ₃ CH ₂ generated Ethene with H ₂ . [CH ₂ =CH ₂] = 4.6x10 ¹⁴ molec.cm ⁻³ . P(Total) = (100-300) torr.	EX	1111-1200	3.98(13)	0	11575	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃CH₂ + D₂ → CH₃CH₂D + D						
Ethyl + Deuterium molecule						
71 BAL/LAN	ES	713	(4.76±0.50)(-2)			2/2
k _{ref} : CH ₃ CH ₂ + CH ₃ CH ₂ CHO → CH ₃ CH ₂ CH ₂ CHO						
71 BAL/LAN	ES	713	8.3(7)			2
CH₃CH₂ + NO → CH₃CH₂NO						
Ethyl + Nitrogen oxide (NO)						
74 PRA/VEL	EX	295	(1.2±0.1)(11)			2
76 PRA/VEL2	EX	325-521	(1.4±0.2)(11)	0	0	2
CH₃CH₂ + CO → CH₃CH₂CO						
Ethyl + Carbon monoxide						
73 WAT/THO	RN	238-378	1.55(11)	0	2416±50	2
CH₃CH₂ + CH₄ → CH₃CH₃ + CH₃						
Ethyl + Methane						
76 CHE/BAC	CO	995	9.0(7)			2
CH₃CH₂ + CH₃CH₂ → CH₂=CH₂ + CH₃CH₃ (a)						
→ CH₃CH₂CH₂CH₃ (b)						
Ethyl						
71 FAL/SUN ¹⁾	RL	298	1.4(-1)			2/2
73 HAR/TAN ¹⁾	RL	298	(1.6±0.4)(-1)			2/2
CH ₂ =CH ₂ photolysis at 163.4 nm.						
73 HAR/TAN ¹⁾	RL	298	(2.1±0.6)(-1)			2/2
CH ₂ =CH ₂ photolysis at 184.9 nm.						
75 HOO/SIM ¹⁾	RL	173-298	1.45(-1)			2/2
77 MAR/MAC ¹⁾	RL	553-673	(1.4±0.3)(-1)			2/2
Thermolysis in a vacuum system.						
79 ADA/BAS3 ¹⁾	RL	298	(1.39±0.13)(-1)			2/2
Flash-photolysis. Absorption-spectroscopy.						
¹⁾ k _a /k _b .						
72 TEN/JON ²⁾	CO	303-603	7.59(12)	0	96	2
Data-fit to a proposed mechanism.						
72 HIA/BEN2 ²⁾	ES	350-410	3.98(11)	0	0±101	2
72 MAR/PUR ²⁾	ES	350-950	2.51(11)	0	0	2
72 PAC/PUR1 ²⁾	DE	951	3.16(11)			2
75 HUG/MAR ²⁾	ES	693-803	2.51(11)	0	0	2
76 GOL/CHO ²⁾	EX	860	4.5(12)			2
Low-pressure k.						
76 PAR/QUI ²⁾	RN	298	(7.83±1.81)(12)			2




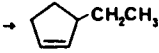
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 ADA/BAS3 ²) Flash-photolysis. Absorption-spectroscopy.	RN	298	(1.24±0.23)(13)			2
80 PAC/WIM2 ²) Ethane pyrolysis in a flow-reactor. Gas-chromatography. P = 100 torr.	ES	903	(1.1±0.4)(13)			2
²) k _b .						
79 ADA/BAS3 k _a + k _b . Flash-photolysis. Absorption spectroscopy.	EX	298	(1.40±0.27)(13)			2
81 COR/MAR k _a + k _b . Ethane pyrolysis in a continuous- flow stirred reactor. Gas-chromatography. P = 40 torr.	EX	803	5.6(12)			2
82 DEM/LES k _a + k _b . Flash-photolysis. Laser Resonance- absorption. CH ₃ CH ₂ generated by flashing NH ₃ in presence of Ethene. Best-fit by simulation.	DE	298	1.2(13)			2
CH₃CH₂ + CH₃CHO → CH₃CH₂CH(O·)CH₃						
Ethyl + Acetaldehyde						
75 BAT/MCC	ES	393-473	7.94(11)	0	0±503	2
CH₃CH₂ + CH₃CH₂NO → (CH₃CH₂)₂NO						
Ethyl + Ethane, nitroso-						
72 TAN/LAM Lower-limit k.	EX	329	≥1.45(10)			2
CH₃CH₂ + CH₃CH₂CHO → CH₃CH₃ + CH₃CH₂CO						
Ethyl + Propanal						
71 BAL/LAN k _{ref} : CH ₃ CH ₂ + H ₂ → CH ₃ CH ₃ + H	RL	713	(8.1±1.0)			2/2
71 BAL/LAN k _{ref} : CH ₃ CH ₂ + D ₂ → CH ₃ CH ₂ D + D	RL	713	(2.1±0.2)(1)			2/2
CH₃CH₂ + CH₂=CHCH₂CH₂ → CH₂=CH₂ + CH₂=CHCH₂CH₃ (a)						
→ CH ₃ CH ₃ + CH ₂ =CHCH=CH ₂ (b)						
→ CH ₂ =CHCH ₂ CH ₂ CH ₂ CH ₃ (c)						
Ethyl + 3-Butenyl						
75 STE/RAB (k _a + k _b)/k _c . Dispr./Comb. ratio.	RL	298	(3.0±0.6)(-1)			2/2





4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)_2$ Ethyl + 1-Propene, 2-methyl- 78 MYS/SHO $\text{CH}_3\text{CH}_2\text{BR}$ ^{60}Co γ -irradiation. Gas-chromatography.	EX	323-423	(1.26±0.04)(5)	0	805±50	2
$\text{CH}_3\text{CH}_2 + \square^{\bullet} \rightarrow \text{CH}_2=\text{CH}_2 + \square$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \square$ (b) $\rightarrow \square\text{CH}_2\text{CH}_3$ (c)						
Ethyl + Cyclobutyl 75 STE/RAB $(k_a + k_b)/k_c$. Dispr./Comb. ratio.	RL	298	(2.3±0.2)(-1)			2/2
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CHCH}_3$ (b)						
Ethyl + Butane 72 PAC/PUR1 ¹⁾ 74 HUG/MAR ¹⁾ Calculation based on experimental data. 76 YAM/NAM ¹⁾ ¹⁾ $k_a + k_b$.	ES DE EX	869-952 895-981 980-1060	3.16(13) 7.94(13) 3.16(12)	0 0 0	10116±856 11162±806 6442±1359	2 2.51 2 2.51 2 3.55
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_2\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{CH}_3\text{CO}$ (c)						
Ethyl + 2,3-Butanedione (Biacetyl) 76 SCH/KNO k_a . 76 SCH/KNO k_b . 76 SCH/KNO k_c .	RN RN RN	525-556 525-556 525-556	2.51(8) 3.98(12) 3.98(8)	0 0 0	3573±302 5385±1560 2969±302	2 2.0 2 15.8 2 2.0
$\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{O} \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_2$ Ethyl + Ethane, 1,1'-oxybis- (Diethyl ether) 77 SER/LAB Diethyl ether/Acetaldehyde pyrolysis. k determined on the basis of a proposed mechanism.	ES	763-823	3.0(11)	0	4026	2




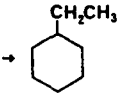
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{S} \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3\text{CHSCH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}_3$ (b) Ethyl + Ethane, 1,1'-thiobis- (Diethyl sulfide)	RN	298-461	(7.4±0.5)(13)	0	3452±49	2
81 EKW/SAF2 k_a . H atoms generated by Hg-photosensitized decomposition of H_2 . Vacuum system. k determined relative to the reaction: $\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{H}_2\text{CH}_3$ P(Diethylsulfide) = (1-32) torr. P(H_2) ~ 580 torr.						
$\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_2\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3$ Ethyl + Diazene, diethyl-	RN	525-556	7.94(11)	0	3775±1359	2 10.0
76 SCH/KNO						
$\text{CH}_3\text{CH}_2 + (\text{CH}_3\text{CH}_2)_2\text{NOH} \rightarrow \text{CH}_3\text{CH}_3 + (\text{CH}_3\text{CH}_2)_2\text{NO}$ Ethyl + Ethanamine, N-ethyl-N-hydroxy-	RN	298	(3.0±0.7)(9)			2
78 ABU/ENC Azoethane photolysis. The abstract gives a rate constant of: $7.2 \times 10^8 \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$, smaller by a factor of 4.4 than the above tabulated k value, which was reported in the text. k determined relative to the reaction: $\text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$. It probably involves abstraction from the hydroxylic Hydrogen.						
$\text{CH}_3\text{CH}_2 + $  $ \rightarrow \text{CH}_2=\text{CH}_2 + $  (a)						
$\rightarrow \text{CH}_3\text{CH}_3 + $  (b)						
$\rightarrow $  (c)						
Ethyl + 2-Cyclopenten-1-yl 75 STE/RAB $(k_a + k_b)/k_c$. Dispr./Comb. ratio.	RL	298	(1.6±0.3)(-1)			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃CH₂ + CH₃CH=CHCH₂CH₂						
→ CH ₃ CH ₃ + cis-CH ₃ CH=CHCH=CH ₂ (a)						
→ CH ₃ CH ₃ + trans-CH ₃ CH=CHCH=CH ₂ (b)						
→ CH ₂ =CH ₂ + cis-CH ₃ CH=CHCH ₂ CH ₃ (c)						
→ CH ₂ =CH ₂ + trans-CH ₃ CH=CHCH ₂ CH ₃ (d)						
→ CH ₃ CH=CHCH ₂ CH ₂ CH ₂ CH ₃ (e)						
Ethyl + 3-Pentenyl						
75 STE/RAB ¹⁾ (k _a + k _b)/k _e .	RL	298	(8.7±1.0)(-2)			2/2
75 STE/RAB ¹⁾ (k _c + k _d)/k _e .	RL	298	(9.3±0.3)(-2)			2/2
¹⁾ Dispr./Comb. ratios.						
CH₃CH₂ + 						
→ CH ₂ =CH ₂ +  (a)						
→ CH ₃ CH ₃ +  (b)						
→  (c)						
Ethyl + Cyclopentyl						
75 STE/RAB (k _a + k _b)/k _c . Dispr./Comb. ratio.	RL	298	(2.6±0.3)(-1)			2/2
CH₃CH₂ + CH₃C(O)C(O)CH₂CH₃						
→ CH ₃ CH ₃ + CH ₂ C(O)C(O)CH ₂ CH ₃ (a)						
→ CH ₃ CH ₃ + CH ₃ C(O)C(O)CHCH ₃ (b)						
→ CH ₃ CH ₃ + CH ₃ C(O)C(O)CH ₂ CH ₂ (c)						
→ (CH ₃ CH ₂) ₂ CO + CH ₃ CO (d)						
Ethyl + 2,3-Pentanedione						
74 SCH/KNO k _b /k _a . T-dependence not detectable.	RL	362-398	≈4.5	0	0	2/2
74 SCH/KNO k _c /k _a . T-dependence not detectable.	RL	362-398	≈3.0(-1)	0	0	2/2
74 SCH/KNO (k _a + k _b + k _c)/k _d .	RL	362-398	5.01(1)	0	1409±1158	2/2 6.31

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2 + $  $ \rightarrow \text{CH}_2=\text{CH}_2 + $  (a)							
$ \rightarrow \text{CH}_3\text{CH}_3 + $  (b)							
$ \rightarrow $  (c)							
Ethyl + Cyclohexyl							
75 STE/RAB	RL	298	$\leq(3.4 \pm 0.5)(-1)$				2/2
$(k_a + k_b)/k_c$.							
Dispr./comb. ratio.							
$\text{CH}_3\text{CH}_2 + \text{CH}_3(\text{CH}_2)_4\text{CH}_3$							
$ \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3(\text{CH}_2)_4\text{CH}_2$							(a)
$ \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3(\text{CH}_2)_3\text{CHCH}_3$							(b)
$ \rightarrow \text{CH}_3\text{CH}_3 + \text{CH}_3(\text{CH}_2)_2\text{CHCH}_2\text{CH}_3$							(c)
Ethyl + Hexane							
76 YAM	RN	973-1088	1.8(13)	0	8052		2
$k_a + k_b + k_c$.							
$\text{CH}_3\text{CH}_3 (+ M) \rightarrow \text{CH}_3 + \text{CH}_3 (+ M)$ (a)							
$ \rightarrow \text{CH}_2=\text{CH}_2 + \text{H}_2 (+ M)$ (b)							
Ethane							
72 PAC/PUR2	EX	920-1040	5.01(16)	0	44505		1
k_a .							
73 BUR/SKI	CO	1000-1500	7.94(16)	0	45043		1
k_a . M = Ar. Limiting high-pressure k.							
RRKM Correlation of experimental data.							
76 CLA/QUI	EX	778-878	1.17(16)	0	43533±252		1 1.38
k_a .							
79 OLS/GAR ¹⁾	CO	1330-2500	7.07(16)	0	45361		1
Extrapolated limiting high-pressure expression							
obtained by applying RRK or RRKM methods to							
the experimental Ethane pyrolysis data from							
79 OLS/TAN.							
79 OLS/GAR ¹⁾	CO	250-2500	2.04(16)	0	44210		1
Limiting high-pressure k, extended to lower							
T-range by combining k's for CH_3 recombination							
at low T, with k's for Ethane decomposition.							
¹⁾ k_a . M = Ar. Decomposition of Ethane behind							
incident shock-waves by Laser-absorption and							
Laser-schlieren experiments.							


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
79 ROT/JUS2 a. Shock-tube. Atomic resonance-absorption. k determined by computer simulation. Total Conc. = (0.2-2.3)x10 ¹⁹ molec.cm ⁻³ .	DE	1450-2100	2.0(15)	0	42000	1	
79 TRE k _a . Thermolysis. P = (3-700) torr.	EX	840-913	5.25(16)	0	44716±342	1	1.48
80 BHA/FRA k _a . Shock-tube. Resonance-absorption. Computer simulation based on a proposed mechanism.	DE	1700-2300	8.0(12)	0	35400	1	
80 PAC/WIM2 k _a . Ethane pyrolysis. Flow-reactor. P = 100 torr.	EX	903	(1.15±0.16)(-5)			1	
81 CHI/SKI2 k _a . M = Ar. Ethane pyrolysis behind reflected shock-waves. Resonance-absorption spectroscopy. k determined relative to the reaction: $\text{CH}_3 + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_4 + \text{CH}_3\text{CH}_2$ P(Total) = (2-3) atm.	RN	1240-1700	2.8(15)	0	42400	1	
81 COR/MAR k _a . Ethane pyrolysis in a continuous-flow stirred tank reactor. Gas-chromatography. P = 40 torr.	EX	840	4.1(-8)			1	
80 BAU/DUX ²⁾ High-pressure k. Critical review.	RE	750-1500	2.40(16)	0	44010±3170	1	3.16
81 BAR ²⁾ Pyrolysis in a quartz reactor.	EX	963-1333	1.55(14)	0	33468	1	
81 BAR ²⁾ Pyrolysis in an inconel reactor.	EX	963-1333	1.0(10)	0	23905±5033	1	
²⁾ k _b .							
71 ILL/WEL ³⁾	EX	993-1097	4.57(15)	0	36633	1	
71 KOR/KAL ³⁾ Pyrolysis in a quartz reactor. Gas-chromatography. P(Total) = 100 torr.	EX	1070-1200	5.0(16)	0	39758	1	1.2
72 ILL/SZA ³⁾	EX	933-1097	6.44(14)	0	34701	1	1.1
74 BAK/NOV ³⁾	EX	973-1123	1.37(16)	0	38853±1510	1	
78 COH ³⁾ Pyrolysis in a flow-reactor.	EX	1040-1190	3.0(16)	0	44288	1	
³⁾ k _{overall} .							
78 VER/BEL ⁴⁾ k _{ref} : CH ₃ CH ₂ CH ₃ → products.	RL	1043-1103	(3.2±0.7)(-1)			1/1	
78 VER/BEL ⁴⁾ k _{ref} : CH ₃ CH ₂ CH ₂ CH ₃ → products.	RL	1023-1193	(1.75±0.15)(-1)			1/1	
⁴⁾ k _{overall} /k _{ref} . Pyrolysis in a flow-reactor.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 IZO/KIS k _a . Shock waves. Best data fit. Total conc.: 5x10 ¹⁷ molec.cm ⁻³ .	DE	1400-2200	2.4(21)	0	44288	2	
79 OLS/TAN k _a . M = Ar. Decomposition behind incident shock-waves. Laser-absorption. Laser-schlieren. Computer simulation by fitting the data to an assumed mechanism with 14 steps. The preexponential factor expressed as: A(T/298) ^{-25.26} .	DE	1300-2500	6.34(48)	-25.26	80320	2	
CH₃CH₃[†] → CH₃ + CH₃							
Ethane							
76 SHI/OBI At 163 nm. CH ₃ CH ₃ [†] formed by CH ₂ [†] + CH ₄ .	EX	298	5.0(9)			1	
76 SHI/OBI At 147 nm. CH ₃ CH ₃ [†] formed by CH ₂ [†] + CH ₄ .	EX	298	6.0(9)			1	
78 LIN/YEH Hg-sensitized photolysis. CH ₃ CH ₃ ^{>} formed by H + CH ₃ CH ₂ . P = (1.5-30) torr.	EX	308	1.7(-7)			1	
CD₃CD₃ → CD₃ + CD₃							
Ethane-d ₆							
76 CLA/QUI	EX	778-878	3.20(16)	0	44269±121	1	1.16
81 CHI/SKI2 M = Ar. Pyrolysis behind reflected shock-waves. Resonance-absorption. k determined relative to the reaction: CD ₃ + CD ₃ CD ₃ → CD ₄ + CD ₃ CD ₂ P(Total) = (2-3) atm.	RN	1240-1700	2.8(15)	0	42400	1	
CH=C=O + O₂ → products							
Ethenyl, 2-oxo- + Oxygen molecule							
73 JON/BAY2 k _{ref} : CH=C=O + O → products.	RL	296	(1.8±0.3)(-2)			2/2	
73 JON/BAY2	RN	296	(2.2±1.2)(10)			2	
CH=C=O + CH≡CH → products							
Ethenyl, 2-oxo- + Ethyne							
73 JON/BAY1 Upper-limit k.	EX	298	<5.0(8)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{C}=\text{O} + \text{CH}_2=\text{C}=\text{O} \rightarrow$ 							
Ethenone (Ketene)							
72 BLA/DAV	EX	498-596	1.78(8)	0	8901±132	2	
$\text{CH}_2=\text{C}=\text{O} + \text{CH}_3\text{COOH} \rightarrow (\text{CH}_3\text{CO})_2\text{O}$							
Ethenone (Ketene) + Acetic acid							
76 BLA/VAY	EX	368-489	1.26(9)	0	6003±114	2	1.29
76 BLA/VAY	EX	428	1.02(3)			2	
$\text{CH}_2=\text{C}=\text{O} + \text{CH}_3\text{CH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}_2\text{COOCOCH}_3$							
Ethenone (Ketene) + Propanoic acid							
76 BLA/VAY	EX	368-489	1.74(9)	0	6102±90	2	1.23
76 BLA/VAY	EX	428	1.12(3)			2	
$\text{CH}_2=\text{C}=\text{O} + \text{CH}_3\text{CH}_2\text{CH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{COOCOCH}_3$							
Ethenone (Ketene) + Butanoic acid							
76 BLA/VAY	EX	428	1.26(3)			2	
$\text{CH}_2=\text{C}=\text{O} + (\text{CH}_3)_2\text{CHCOOH} \rightarrow (\text{CH}_3)_2\text{CHCOOCOCH}_3$							
Ethenone (Ketene) + Propanoic acid, 2-methyl-							
76 BLA/VAY	EX	428	1.57(3)			2	
$\text{CH}_2=\text{C}=\text{O} + (\text{CH}_3)_3\text{CCOOH} \rightarrow (\text{CH}_3)_3\text{CCOOCOCH}_3$							
Ethenone (Ketene) + Propanoic acidm 2,2-dimethyl-							
76 BLA/VAY	EX	368-489	1.55(9)	0	5754±100	2	1.26
76 BLA/VAY	EX	428	2.23(3)			2	
$\text{CH}_2=\text{C}=\text{O} + (\text{CH}_3)_3\text{CCH}_2\text{COOH} \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{COOCOCH}_3$							
Ethenone (Ketene) + Butanoic acid, 3,3-dimethyl-							
76 BLA/VAY	EX	428	1.63(3)			2	
$\text{CH}_3\text{CO} (+ \text{M}) \rightarrow \text{CH}_3 + \text{CO} (+ \text{M})$							
Ethyl, 1-oxo- (Acetyl)							
73 FRE/VIN	RN	326	(1.91±0.3)(1)			1	
Estimated k on the basis of a proposed mechanism.							
74 SZI/WAL ¹⁾	RL	507	(2.41±0.34)(-8)			1/2	
k _{ref} : CH ₃ CO + HI → CH ₃ CHO + I							
74 SZI/WAL ¹⁾	RN	498-525	2.00(13)	0	10970±902	1	3.16
Estimated, limiting high-pressure k.							
¹⁾ M = N ₂ , or cy-(CF ₂) ₄ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 WAT/WOR	RN	333-413	1.58(13)	0	8661±241	1	2.0
82 ANA/MAW ²⁾	EX	323	(2.45±0.74)(1)			1	
82 ANA/MAW ²⁾	EX	343	(1.86±0.56)(2)			1	
Limiting high-pressure k.							
82 ANA/MAW ²⁾	EX	343	(1.87±0.56)(7)			2	
Limiting low-pressure k.							
²⁾ M = CO. Molecular modulation spectroscopy.							
CH ₃ CO produced by Azomethane/CO photolysis.							
[Azomethane] = 1.0x10 ¹⁷ molec.cm ⁻³ .							
[CO] = (0.3-2.7)x10 ¹⁹ molec.cm ⁻³ .							
CH ₃ CO + O ₂ → CH ₃ C(O)O ₂							
Ethyl, 1-oxo- (Acetyl) + Oxygen molecule							
74 DIX/SKI1	ES	336-357	(1.2±0.3)(10)			2	
82 MCD/LEN	EX	298	(1.20±0.24)(12)			2	
CH ₃ CO generated by Photolysis of Acetone, or Acetyl-Acetone vapor in (1-4) torr. He.							
CH ₃ CO + NO → products							
Ethyl, 1-oxo- (Acetyl) + Nitrogen oxide (NO)							
82 MCD/LEN	EX	298	(5.60±1.63)(11)			2	
CH ₃ CO generated by Photolysis of Acetone, or Acetylacetone vapor, in (1-4) Torr He.							
CH ₃ CO + NO ₂ → CH ₃ CO ₂ + NO							
Ethyl, 1-oxo- (Acetyl) + Nitrogen oxide (NO ₂)							
82 SLA/GUT	EX	295	(1.51±0.36)(13)			2	
Flow-reactor. CH ₃ CO generated by reacting Cl atoms with CH ₃ CHO. Cl atoms generated by IR- multiphoton-induced decomposition of CF ₂ Cl ₂ . [CH ₃ CO] ₀ = (1.9-4.6)x10 ¹⁰ molec.cm ⁻³ . [CH ₃ CHO] = (5.7-6.5)x10 ¹⁴ molec.cm ⁻³ . [NO ₂] = (0-5)x10 ¹² molec.cm ⁻³ . P = (1-20) torr.							
CH ₃ CO + CH ₃ CO → CH ₃ C(O)C(O)CH ₃ (a)							
→ (CH ₃) ₂ CO + CO (b)							
→ CH ₃ CHO + CH ₂ =C=O (c)							
Ethyl, 1-oxo- (Acetyl)							
79 HAS/KOS	EX	298	2.37(13)			2	
k _a . CH ₃ OOCH ₃ Flash-photolysis. Gas-chromatography. P = (1.5-700) torr.							


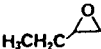



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 PAR k _a . Photolysis of Acetone at (25.4-40.0) nm. Molecular modulation spectroscopy.	EX	298	(1.81±0.60)(13)			2
82 ANA/MAW k _a . Average of 24 k values obtained through a data-fit procedure. Molecular Modulation Spectroscopy. CH ₃ and CH ₃ CO produced by Azomethane/CO photolysis. P-independent k. [Azomethane] = 1.0x10 ¹⁷ molec.cm ⁻³ . [CO] = (0.3-2.7)x10 ¹⁹ molec.cm ⁻³ .	EX	263-343	(7.23±1.81)(12)	0	0	2
82 TIM/KAL k _a . 2,3-Butanedione flash-photolysis. Gas-chromatography. [CH ₃ CO] = (1.14-5.77)x10 ¹⁸ molec.cm ⁻³ . P = (11-47) torr.	EX	298	(2.43±0.14)(13)			2
78 ADA/BAS k _a + k _b + k _c . Acetone Flash-photolysis. Kinetic Spectroscopy. P(Total) = 50 torr.	ES	298	4.5(13)			2
81 ADA/BAS2 k _a + k _b + k _c . Acetone Flash-photolysis. Kinetic Spectroscopy.	ES	298	3.5(13)			2
CD ₃ CO + CD ₃ CO → CD ₃ C(O)C(O)CD ₃ (a) → (CD ₃) ₂ CO + CO (b) → CD ₃ CDO + CD ₂ =C=O (c)						
Ethyl-2,2,2-d ₃ , 1-oxo- (Acetyl)						
81 ADA/BAS2 k _a + k _b + k _c . Acetone-d ₆ Flash-photolysis. Kinetic Spectroscopy.	ES	298	3.4(13)			2
CH ₃ CO + CH ₃ CHO → (CH ₃) ₂ CO + CHO Ethyl, 1-oxo- (Acetyl) + Acetaldehyde						
81 GIL/JOH Flash-photolysis of CH ₃ CHO. Time-resolved intracavity laser detection. P(CH ₃ CHO) = 0.2 torr.	EX	298	(1.71±0.37)(11)			2
CH ₃ CO + CH ₂ =CHCH=CH ₂ → CH ₃ C(O)CH ₂ CHCH=CH ₂ Ethyl, 1-oxo- + 1,3-Butadiene						
73 ENC/LIS k _{ref} : CH ₃ CO (+M) → CH ₃ + CO (+M)	RL	333-397	1.6(3)	0	-5284±503	2/1 5.01

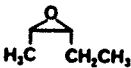
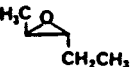
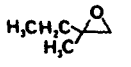

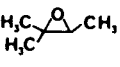
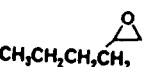
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃C(O)O + NO₂ → CH₃C(O)O₂NO₂							
Ethoxy, 1-oxo- + Nitrogen oxide (NO ₂)							
77 HEN/KEN	ES	298-318	6.3(11)	0	0	2	
CH₃C(O)OO + NO → CH₃ + CO₂ + NO₂ (a)							
→ CH ₃ C(O)O + NO ₂ (b)							
Ethyldioxy, 1-oxo- + Nitrogen oxide (NO)							
76 COX/DER3	RL	296	(1.73±0.006)			2/2	
k _a /k _{ref} .							
k _{ref} : CH ₃ C(O)OO + NO ₂ → CH ₃ C(O)OONO ₂							
77 HEN/KEN	RL	298-318	(3.1±0.5)	0	0	2/2	
k _b /k _{ref} .							
k _{ref} : CH ₃ C(O)OO + NO ₂ → CH ₃ C(O)OONO ₂							
77 COX/ROF ¹⁾	ES	300	1.63(12)			2	
77 HEN/KEN ¹⁾	RN	298-318	2.0(12)	0	0	2	
¹⁾ k _b .							
CH₃C(O)OO + NO₂ → CH₃C(O)OONO₂ (a)							
→ any other products (b)							
Ethyldioxy, 1-oxo- + Nitrogen oxide (NO ₂)							
77 COX/ROF ¹⁾	RL	303-328	≈(5.4±1.7)(-1)			2/2	
k _a /k _{ref} .							
Mean rate ratio.							
k _{ref} : CH ₃ C(O)OO + NO → CH ₃ C(O)O + NO ₂							
77 COX/ROF ¹⁾	DE	300	8.43(11)			2	
k _a .							
Based on k/k _{ref} and Thermodynamic data.							
¹⁾ Thermolysis in a flow-reactor.							
80 ADD/BUR ²⁾	EX	302	(1.26±0.06)(12)			2	
P = 28 torr.							
80 ADD/BUR ²⁾	EX	302	(2.83±0.18)(12)			2	
P = 715 torr.							
²⁾ k _a .							
Cl ₂ /CH ₃ CHO/O ₂ Modulated Photolysis.							
77 COX/DER3	RL	298	(2.4±1.4)(-1)			2/2	
k _{overall} /k _a .							
CH₃C(O)OO + HCHO → CH₃C(O)OOH + CHO							
Ethyldioxy, 1-oxo- + Formaldehyde							
74 DIX/SKI2	RL	392-461	(2.4±0.2)	0	0	2/2	
Rate-ratio assumed to be T-independent.							
k _{ref} :							
CH ₃ C(O)OO + CH ₃ CHO → CH ₃ C(O)OOH + CH ₃ CO							


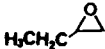

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{C}(\text{O})\text{OO}$ → $\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 + \text{CO}_2 + \text{CO}_2 + \text{O}_2$ (a) → any other products (b)							
Ethylidioxy, 1-oxo-							
80 ADD/BURR ¹⁾ k_a . Data-fit by computer simulation on the basis of a proposed mechanism.	DE	302	1.51(12)			2	2.0
80 ADD/BURR ¹⁾ k_{overall} . Weighted least-squares fit by assuming a simple second-order rate law.	EX	302	(3.9±1.8)(12)			2	
¹⁾ $\text{Cl}_2/\text{CH}_3\text{CHO}/\text{O}_2$ modulated photolysis.							
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CO}_2 +$ 							
Ethylidioxy, 1-oxo- + 1-Propene							
77 DIA/SEL	RN	393	(6.40±0.36)(6)			2	
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CO}_2 +$ 							
Ethylidioxy, 1-oxo- + 1-Butene							
74 DIA/WAD	RN	393	3.5(7)			2	
75 SEL/WAD	RN	357-410	8.7(10)	0	3480±422	2	3.0
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$ → $\text{CH}_3 + \text{CO}_2 +$ 							
Ethylidioxy, 1-oxo- + 2-Butene, (Z)-							
72 RAY/WAD	ES	457	2.0(9)			2	
75 DIA/SEL	RN	393	(7.5±0.1)(7)			2	
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$ → $\text{CH}_3 + \text{CO}_2 +$ 							
Ethylidioxy, 1-oxo- + 2-Butene, (E)-							
75 DIA/SEL	RN	393	(1.2±0.1)(8)			2	
$\text{CH}_3\text{C}(\text{O})\text{OO} + (\text{CH}_3)_2\text{C}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CO}_2 +$ 							
Ethylidioxy, 1-oxo- + 1-Propene, 2-methyl-							
75 SEL/WAD	RN	357-410	1.9(11)	0	3012±141	2	



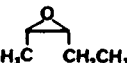
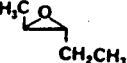
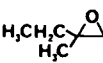
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A	k _{err}
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{cis-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$  Ethyldioxy, 1-oxo- + 2-Pentene, (Z)- 77 DIA/SEL	RN	393	(1.41±0.84)(8)				2
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{trans-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$  Ethyldioxy, 1-oxo- + 2-Butene, (E)- 77 DIA/SEL	RN	393	(1.41±0.84)(8)				2
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$  Ethyldioxy, 1-oxo- + 1-Butene, 2-methyl- 74 DIA/WAD 77 DIA/SEL	RN	393	5.0(8)				2
$\text{CH}_3\text{C}(\text{O})\text{OO} + (\text{CH}_3)_2\text{CHCH}=\text{CH}_2$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$  Ethyldioxy, 1-oxo- + 1-Butene, 3-methyl- 77 DIA/SEL	RN	393	(1.25±0.62)(7)				2
$\text{CH}_3\text{C}(\text{O})\text{OO} + (\text{CH}_3)_2\text{C}=\text{CHCH}_3$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$  Ethyldioxy, 1-oxo- + 2-Butene, 2-methyl- 77 DIA/SEL 77 DIA/SEL	RN	370-410 393	1.21(11) (8.38±0.84)(8)	0	1965±109		2 2 1.31
$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ $\rightarrow \text{CH}_3 + \text{CO}_2 +$  Ethyldioxy, 1-oxo- + 1-Hexene 77 DIA/SEL	RN	393	(2.24±0.83)(7)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CHO (+ M) → CH₃ + CHO (+ M)							
Acetaldehyde							
73 BAR/MAR M = H ₂ . Based on analytical data.	EX	768-813	(3.88±2.94)(16)	0	40106±695	1	
73 BAR/MAR M = H ₂ . Based on pressure-time data.	EX	768-813	(8.87±4.42)(16)	0	41012±1636	1	
75 COL/NAE M = N ₂ .	EX	800-1225	7.08(15)	0	41155±503	1	1.62
76 ERN/SFI M = Ar. Limiting high-pressure k.	EX	1350-1650	1.2(16)	0	41137±481	1	
CH₃CHO + CH₃C(O)OOH → products							
Acetaldehyde + Ethaneperoxy acid							
74 DIX/SKI1 ¹⁾	RN	336	2.0(-1)				2
74 DIX/SKI1 ¹⁾	RN	345	1.9(-1)				2
74 DIX/SKI1 ¹⁾	RN	393	4.45				2
¹⁾ Surface/volume ratio = 0.6 cm ⁻¹ .							
74 DIX/SKI1 ²⁾	RN	345	7.3(-1)				2
74 DIX/SKI1 ²⁾	RN	393	2.1(2)				2
²⁾ Surface/volume ratio = 6.1 cm ⁻¹ .							
CH₃C(O)OOH + CH₃CH=CH₂ → CH₃COOH + 							
Ethaneperoxy acid + 1-Propene							
77 DIA/SEL	RN	393	(2.32±0.86)				2
CH₃C(O)OOH + CH₃CH₂CH=CH₂							
→ CH₃COOH + 							
Ethaneperoxy acid + 1-Butene							
75 SEL/WAD	RN	357-410	4.8(11)	0	9915±1241	2	25.0
CH₃C(O)OOH + cis-CH₃CH=CHCH₃							
→ CH₃COOH + 							
Ethaneperoxy acid + 2-Butene, (Z)-							
75 DIA/SEL Alkene added after CH ₃ CHO consumption.	RN	393	(3.0±0.7)(1)				2
75 DIA/SEL Alkene added at the start of CH ₃ CHO + O ₂ reaction.	RN	393	(3.4±1.0)(1)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{trans-CH}_3\text{CH}=\text{CHCH}_3$ $\rightarrow \text{CH}_3\text{COOH} + $ 						
Ethaneperoxy acid + 2-Butene, (E)-						
75 DIA/SEL Alkene added after CH_3CHO consumption.	RN	393	(3.0±0.7)(1)			2
75 DIA/SEL Alkene added at the start of $\text{CH}_3\text{CHO} + \text{O}_2$ reaction.	RN	393	(3.4±1.0)(1)			2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} + $ 						
Ethaneperoxy acid + 1-Propene, 2-methyl-						
75 SEL/WAD	RN	357-410	4.3(10)	0	7939±1629	2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{cis-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3$ $\rightarrow \text{CH}_3\text{COOH} + $ 						
Ethaneperoxy acid + 2-Pentene, (Z)-						
77 DIA/SEL	RN	393	(4.28±1.70)			2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{trans-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_3$ $\rightarrow \text{CH}_3\text{COOH} + $ 						
Ethaneperoxy acid + 2-Pentene, (E)-						
77 DIA/SEL	RN	393	(4.38±1.70)			2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} + $ 						
Ethaneperoxy acid + 1-Butene, 2-methyl-						
77 DIA/SEL	RN	393	(6.03±2.16)(1)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{O})\text{OOH} + (\text{CH}_3)_2\text{C}=\text{CH}-\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} + \text{Cyclopropane ring with } (\text{CH}_3)_2\text{CH}$						
Ethaneperoxoic acid + 1-Butene, 3-methyl-						
77 DIA/SEL	RN	393	(9.97±2.10)			2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + (\text{CH}_3)_2\text{C}=\text{CHCH}_3$ $\rightarrow \text{CH}_3\text{COOH} + \text{Cyclopropane ring with } \text{H}_3\text{C}$						
Ethaneperoxoic acid + 2-Butene, 2-methyl-						
77 DIA/SEL	RN	370-410	1.70(11)	0	7410±291	2 2.14
77 DIA/SEL	RN	393	(1.24±0.15)(3)			2
$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} + \text{Cyclopropane ring with } \text{CH}_2\text{CH}_2\text{CH}_2$						
Ethaneperoxoic acid + 1-Hexene						
77 DIA/SEL	RN	393	(2.13±1.20)(1)			2
$\text{CH}_3\text{CH}_2\text{O} \rightarrow \text{CH}_3 + \text{HCHO}$ (a) $\rightarrow \text{CH}_3\text{CHO} + \text{H}$ (b)						
Ethoxy						
74 MOS/POL	RL	593	(1.4±0.2)(5)			1/2
k_{ref} : $\text{CH}_3\text{CH}_2\text{O} + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{OH} + \text{CH}_2\text{CH}_3$						
77 BAT/MIL2 1)	ES	435-491	1.0(15)	0	10871	1
79 BAT 1)	ES	393-473	1.0(15)	0	10871±503	1 3.16
1) k_a . Conventional static system.						
77 BAT/MIL2 2)	ES	435-491	2.51(14)	0	9763	1
79 BAT 2)	ES	393-473	2.51(14)	0	11778	1
2) k_b . Conventional static system.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CH₂O + O₂ → CH₃CHO + HO₂							
Ethoxy + Oxygen molecule							
82 GUT/SAN ¹⁾	EX	296	4.8(9)			2	
82 GUT/SAN ¹⁾	EX	353	5.9(9)			2	
¹⁾ CH ₃ CH ₂ ONO photolysis at 266 nm. Laser-induced Fluorescence. P(O ₂ + N ₂) = 40 torr.							
CH₃CH₂O + NO → CH₃CHO + HNO (a) → CH₃CH₂ONO (b)							
Ethoxy + Nitrogen oxide (NO)							
77 BAT/MIL2	ES	435-491	6.31(12)	0	0±503	2	2.51
k _a .							
80 ROS	RL	298	(0.18±0.02)			2/2	
k _a /k _{ref} . CH ₃ CH ₂ NO ₂ /NO ₂ photolysis at 366 nm. k _{ref} : CH ₃ CH ₂ O + NO → CH ₃ CH ₂ ONO							
77 BAT/MIL2	ES	435-491	2.0(13)	0	0±503	2	2.51
k _b . Same data in 74 BAT/MIL and 75 BAT/MCC.							
CH₃CH₂O + NO₂ → CH₃CHO + HONO (a) → CH₃CH₂ONO₂ (b)							
Ethoxy + Nitrogen oxide (NO ₂)							
77 BAT/MIL2	ES	435-491	3.98(12)	0	0	2	
k _a .							
80 ROS	RL	298	(9.0±1.0)(-2)			2/2	
k _a /k _b . CH ₃ CH ₂ NO ₂ /NO ₂ photolysis at 366 nm.							
77 BAT/MIL2	ES	435-491	7.94(12)	0	0	2	
k _b .							
CH₃CBOH (+ M) → CH₃CHO + H (+ M)							
Ethyl, 1-hydroxy-							
82 NAT/BHA	ES	1300-1700	5.00(13)	0	11000	2	
M = O ₂ + Ar. Ethanol/O ₂ /Ar ignition behind reflected shock-waves. Data-fit. P = (1-2) atm.							
CH₃CBOH + O₂ → CH₃CHO + HO₂ (a) → CH₃CH(OH)OO (b)							
Ethyl, 1-hydroxy- + Oxygen molecule							
82 NAT/BHA	ES	1300-1700	1.00(13)	0	2800	2	
k _a . M = O ₂ + Ar. Ethanol/O ₂ /Ar ignition behind reflected shock-waves. Data-fit. P = (1-2) atm.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes.	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
81 WAS k _{overall} . Fast-flow reactor. Photoionization Mass-spectrometry. P(Ethanol) = 1.15 mtorr. P(Total) = 3.73 mtorr. P(O) _o = 9.78 mtorr. P(O) = 9.42 mtorr. k _{ref} : CD ₃ CDOH + ¹⁸ O → CD ₃ CDO + ¹⁸ OH (c) → CD ₃ CD ¹⁸ O → OH (d)	RL	298	(1.4±0.4)(-1)				2/2
CH ₃ CH ₂ O ₂ → HCHO + CH ₃ O (a) → CH ₃ CHO + OH (b) → CH ₂ CH ₂ OOH (c)							
Ethyldioxy							
74 MOS/POL k _a /k _b .	RL	593	1.34(1)				1/1
80 BAL/FIC k _c . Static system. Gas-chromatography.	ES	673-813	1.94(13)	0	17285±1208	1	3.16
CH ₃ CH ₂ O ₂ + NO → CH ₃ CH ₂ O + NO ₂ Ethyldioxy + Nitrogen oxide (NO)							
79 ADA/BAS5 Azoethane/O ₂ /Ar photolysis. Kinetic-spectroscopy. [Azoethane] = (2.2-6.6)×10 ¹⁶ molec.cm ⁻³ . [O ₂] = (2.0-3.3)×10 ¹⁷ molec.cm ⁻³ . [Ar] = (1.1-2.5)×10 ¹⁸ molec.cm ⁻³ . [NO] = (0.2-2.1)×10 ¹⁵ molec.cm ⁻³ . Flash energy = 263cal.(1.1kJ).	EX	298	(1.6±0.1)(12)				2
82 PLU/RVA1 Flow-reactor. M = He. Mass-spectrometry. CH ₃ CH ₂ O ₂ generated by reacting Cl ₂ with CH ₃ CH ₃ and O ₂ in He, in a microwave discharge. [He] = 1.6×10 ¹⁷ molec.cm ⁻³ .	EX	295	(5.36±1.81)(12)				2
CH ₃ CH ₂ O ₂ + NO ₂ → products Ethyldioxy + Nitrogen oxide (NO ₂)							
79 ADA/BAS2 Flash-photolysis. Kinetic-spectroscopy. [Azoethane] < 3.0×10 ¹⁷ molec.cm ⁻³ . [Ar] ~ 1.2×10 ¹⁸ molec.cm ⁻³ . [O ₂] < 2.2×10 ¹⁹ molec.cm ⁻³ .	EX	298	(7.48±0.39)(11)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data	T/K	k, k/k(ref),	n	B,	k, A	k err.
$\text{CH}_3\text{CH}_2\text{O}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{O} + \text{C}_2\text{H}_4$							
Ethyldioxy + Ethene							
78 MOS/POL ¹⁾	ES	593	2.0(8)				2
78 MOS/POL ¹⁾	DE	653	1.1(9)				2
¹⁾ Static reactor.							
Gas-chromatography.							
Based on calculated $\text{CH}_3\text{CH}_2\text{O}_2$ concentrations.							
$\text{CH}_3\text{CH}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{O} + \text{CH}_3\text{CH}_2\text{O} + \text{O}_2$ (a)							
$\rightarrow \text{CH}_3\text{CHO} + \text{CH}_3\text{CH}_2\text{OH} + \text{O}_2$ (b)							
$\rightarrow \text{CH}_3\text{CH}_2\text{OOCH}_2\text{CH}_3 + \text{O}_2$ (c)							
Ethyldioxy							
79 ADA/BAS4	DE	298	(6.0±0.6)(10)				2
$k_a + k_b + k_c$.							
Flash-photolysis.							
Absorption-spectroscopy							
Computer data-fit.							
82 NIK/MAK2 ¹⁾	RL	298	1.3				2/2
k_a/k_b .							
82 NIK/MAK2 ¹⁾	RL	298	≤2.2(-1)				2/2
k_c/k_b .							
¹⁾ FTIR-Spectroscopy.							
$\text{CH}_3\text{CH}_2\text{O}_2$ generated by photolysis							
of an Azoethane/ O_2/N_2 mixture.							
[Azoethane] = 6.15×10^{14} molec. cm^{-3} .							
$P(\text{N}_2) = 650$ torr.							
$P(\text{O}_2) = 50$ torr.							
$\text{CH}_3\text{CH}_2\text{OH} (+ \text{M}) \rightarrow \text{CH}_3 + \text{CH}_2\text{OH} (+ \text{M})$							
Ethanol							
76 TSA1	ES	1080-1165	2.51(6)	0	42500		1
82 NAT/BHA	CO	1300-1700	3.00(18)	0	38000		2
$\text{M} = \text{O}_2 + \text{Ar}$.							
Ethanol/ O_2/Ar ignition behind							
reflected shock-waves.							
Data-fit.							
$P = (1-2)$ atm.							
$(\text{CH}_3)_2\text{O} \rightarrow \text{CH}_3\text{O} + \text{CH}_3$							
Methane, oxybis- (Dimethyl ether)							
75 PAC	EX	782-936	1.0(15)	0	38251±962	1	3.16
77 ARO/NAE1	EX	1063-1223	2.16(15)	0	38551	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 HEL/MAN Pyrolysis in a flow-reactor. UV-absorption-spectroscopy. Computer simulation. High-pressure k.	DE	1005	3.1(-2)			1	
78 ARO Pyrolysis in a flow reactor.	EX	1062-1223	2.16(15)	0	38551	1	
82 BAT/ALV (CH ₃) ₂ O pyrolysis with, or without CH ₄ . Static system. P(CH ₃ OCH ₃) = (400-800) torr.	EX	680-850	3.16(16)	0	41772±1007	1	6.31
CH₃OOCH₃ → CH₃O + CH₃O							
Peroxide, dimethyl-							
73 LIS/MAS	ES	400	3.3(-4)			1	
76 BAT/MCC1	EX	383-413	3.16(15)	0	18621±101	1	3.16
77 BAR/BEN1 Vacuum technique. Gas-chromatography.	EX	391-432	5.01(15)	0	18671±453	1	3.16
79 BAT/RAT ¹) k determined in presence of NO and CF ₄ .	EX	383-420	7.94(13)	0	16960±554	1	3.98
79 BAT/RAT ¹) k determined in presence of NO and NO ₂ .	EX	383-433	2.51(16)	0	19376±302	1	1.58
¹) Static system, with packed reaction vessels.							
△^S → CH₂=CH₂ + S							
Thiirane (Ethylene episulfide)							
82 AMA/YAM VLP-Pyrolysis. P < 10 ⁻⁵ torr.	EX	1030-1100	6.31(15)	0	21339	1	
△^S → CH₂=CHSH							
Thiirane (Ethylene episulfide)							
79 SHE/SAF ¹) k determined by experimental kinetics.	EX	298	5.0(10)			1	
79 SHE/SAF ¹) k calculated by RRKM theory.	CO	298	7.6(10)			1	
¹) COS UV-photolysis. High-vacuum system. Thiirane is in a vibrationally excited singlet ground state formed by S(¹ D ₂) + CH ₂ =CH ₂ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{SCH}_2 + \text{CH}_4 \rightarrow (\text{CH}_3)_2\text{S} + \text{CH}_3$ Methyl, (methylthio)- + Methane							
76 ART/LEE Calculation based on the reverse reaction and Thermochemical data.	DE	393-518	6.31(1)	0	7662	2	
$\text{NCCN} (+ \text{M}) \rightarrow \text{CN} + \text{CN} (+ \text{M})$ Ethane dinitrile							
73 FUE/TAB M = Ar.	EX	2200-3700	(6.66±1.25)(16)	0	49643±609	2	
$\text{CH}_3\text{NC} \rightarrow \text{CH}_3\text{CN}$ Methane, isocyano-							
76 COL/PRI Thermal isomerization in static vessels. P = (2-100) torr.	EX	393-593	2.24(13)	0	19225±101	1	1.3
$(\text{CH}_3)_2\text{N} + \text{O}_2 \rightarrow \text{CH}_2=\text{NCH}_3 + \text{HO}_2$ Amidogen, dimethyl- + Oxygen molecule							
79 LIN/CAL ¹⁾ $k_{\text{ref}}: (\text{CH}_3)_2\text{N} + \text{NO} \rightarrow (\text{CH}_3)_2\text{NN}=\text{O}$	RL	298	(1.48±0.07)(-6)				2/2
79 LIN/CAL ¹⁾ $k_{\text{ref}}: (\text{CH}_3)_2\text{N} + \text{NO}_2 \rightarrow (\text{CH}_3)_2\text{NNO}_2$	RL	298	(3.90±0.28)(-7)				2/2
¹⁾ Long-path, FTIR-spectroscopy.							
$(\text{CH}_3)_2\text{N} + \text{NO}_2 \rightarrow \text{CH}_2=\text{NCH}_3 + \text{HONO}$ (a) $\rightarrow (\text{CH}_3)_2\text{NNO}_2$ (b) Amidogen, dimethyl- + Nitrogen oxide (NO ₂)							
79 LIN/CAL k_a/k_b . Long-path, FTIR-Spectroscopy.	RL	298	(2.2±0.6)(-1)				2/2
$\text{CH}_3\text{N}=\text{NCH}_3 \rightarrow \text{CH}_3 + \text{CH}_3 + \text{N}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_3 + \text{N}_2$ (b) Diazene, dimethyl- (Azomethane)							
75 CAM/MAR k_a .	EX	676-813	2.00(13)	0	22734±481	1	2.0
78 MAR/PAG ¹⁾ k_a .	EX	534-657	7.94(13)	0	23287±301	1	1.66

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 MAR/PAG ¹⁾ k _b . ¹⁾ Azomethane pyrolysis in a static vacuum system. P = (50-150) torr.	EX	534-657	3.39(11)	0	22193±854	1	3.89
$\text{CH}_3\text{N}=\text{NCH}_3^* \rightarrow \text{CH}_3 + \text{CH}_3 + \text{N}_2$ Diazene, dimethyl- (Azomethane)							
77 CHE/ORE Azomethane/He high-P photolysis. RRKM data-fit to a proposed mechanism. Azomethane assumed to be in a vibrationally excited T ₁ electronic state. Lower-limit k. (He) = (0-100) atm.	CO	298	>4.0(10)			1	
$(\text{CH}_3)_2\text{NNH}_2 \rightarrow (\text{CH}_3)_2\text{N} + \text{NH}_2$ Hydrazine, 1,1-dimethyl-							
72 GOL/SOL RRKM fit of experimental data.	EX	869-1076	3.98(17)	0	31706	1	
$\text{CH}_3\text{NHNHCH}_3 \rightarrow \text{CH}_3\text{N}=\text{NCH}_3 + \text{H}_2$ Hydrazine, 1,2-dimethyl-							
72 GOL/SOL RRKM fit of experimental data.	EX	910-1271	3.16(13)	0	28686	1	
$\text{CH}_3\text{COOONO}_2 \rightarrow \text{CH}_3\text{COOO} + \text{NO}_2$ Peroxide, acetyl nitro-							
77 COX/ROF Thermolysis in a flow reactor.	EX	294-328	7.94(14)	0	12510±385	1	3.98
77 HEN/KEN	EX	298-313	1.95(16)	0	13543±453	1	3.98
77 HEN/KEN	EX	298	(4.0±0.9)(-4)			1	
$\text{CH}_3\text{CH}_2\text{NO} + \text{CH}_3\text{CH}_2\text{NO} \rightarrow (\text{CH}_3\text{CH}_2\text{NO})_2$ Ethane, nitroso-							
72 TAN/LAM	EX	314	(3.01±0.30)(4)			2	
$\text{CH}_3\text{CH}_2\text{NO}_2 (+ \text{M}) \rightarrow \text{CH}_3\text{CH}_2 + \text{NO}_2 (+ \text{M})$ Ethane, nitro-							
73 GLA/TRO ¹⁾ Limiting high-pressure k.	EX	900-1350	7.94(15)	0	28686	1	
73 GLA/TRO ¹⁾ Limiting low-pressure k.	EX	900-1350	1.0(18)	0	18118	2	
¹⁾ Thermolysis in shock waves. Conc.(Ar): (0.027-1.807)10 ²⁰ molec.cm ⁻³ .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃CH₂ONO → CH₃CHO + HNO (a)						
→ CH₃CH₂O + NO (b)						
Nitrous acid ethyl ester (Ethyl nitrite)						
75 BAT/MCC ¹⁾	ES	393-473	6.31(13)	0	18873	1
77 BAT/MIL2 ¹⁾	ES	435-491	5.01(13)	0	18873	1
78 BAT/ISL2 ¹⁾	EX	433-473	7.94(14)	0	20081±503	1 3.16
Pyrolysis in a static system.						
Gas-chromatography.						
¹⁾ k _a .						
77 BAT/MIL2	ES	435-491	1.0(16)	0	21037±453	1 2.51
k _b .						
Same data given in 74 BAT/MIL and 75 BAT/MCC.						
CH₃CH₂ONO₂ → CH₃CH₂ + NO₂						
Nitric acid ethyl ester (Ethyl nitrate)						
77 BAT/MIL2	ES	435-491	1.0(16)	0	20131	1
C₃ + O₂ → C₂(d³Π, v=1) + CO + O (or CO₂) (a)						
→ any other product (b)						
Carbon trimer + Oxygen molecule						
77 MAN	EX	2470	≥1.20(12)			2
k _a . High-T flowing system.						
Lower-limit k.						
80 LES/HIC	EX	298	≤9.03(9)			2
k _{overall} . Laser-induced fluorescence.						
Upper-limit k.						
80 REI/MAN1	EX	300	≤1.20(10)			2
k _{overall} . Upper-limit k.						
IR Multiphoton dissociation of Allene.						
82 NEL/HEL	EX	295-610	≤1.20(8)			2
k _{overall} . C ₃ generated by multiphoton						
UV-photolysis of C ₆ H ₆ at 249 nm.						
Laser-induced Fluorescence.						
Upper-limit k.						
P(Total) = (5-100) torr.						
P(C ₆ H ₆) = (1-2) mtorr.						
P(O) = 90 torr.						
C₃ + N₂ → products						
Carbon trimer + Nitrogen molecule						
80 REI/MAN1	EX	300	≤1.81(10)			2
IR-Multiphoton dissociation of Allene.						
Upper-limit k.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
C₃ + NO → products						
Carbon trimer + Nitrogen oxide (NO)						
80 LES/HIC Dye-laser induced fluorescence.	EX	298	1.26(11)			2
80 REI/MAN1 IR Multiphoton dissociation of 1,2-Propadiene. Upper-limit k.	EX	300	≤1.81(10)			2
C₃ + CH₄ → products						
Carbon trimer + Methane						
80 REI/MAN1 IR-Multiphoton dissociation of Allene. Upper-limit k.	EX	300	≤1.81(10)			2
82 NEL/HEL C ₃ generated by Multiphoton Laser-photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. Upper-limit k. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr. P(CH ₄) = 90 torr.	EX	295-610	≤3.01(8)			2
C₃ + CH=CH → products						
Carbon trimer + Ethyne						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser photolysis of C ₆ H ₆ . Laser-induced Fluorescence. Upper-limit k. P(CH=CH) = (0-50) torr.	EX	294	<6.02(8)			2
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. Probable Products: C ₃ H + CH=C. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr. P(CH=CH) = (0-30) torr.	EX	295-610	(5.47±1.61)(12)	0	4065±161	2
C₃ + CH₂=CH₂ → products						
Carbon trimer + Ethene						
81 NEL/PAS C ₃ is generated by multiphoton UV excimer laser photolysis of C ₆ H ₆ . Laser-induced Fluorescence. Upper-limit k. P(CH ₂ =CH ₂) = (0-68) torr.	EX	294	<6.02(8)			2
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. Probable products: C ₃ H + CH ₂ =CH. P(Total) = (5-100) torr. P(CH ₂ =CH ₂) = (0-50) torr. P(C ₆ H ₆) = (1-2) torr.	EX	295-610	(1.03±0.31)(12)	0	3277±168	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C₃ + CH₃CH₃ → products						
Carbon trimer + Ethane						
80 REI/MAN1 IR-Multiphoton dissociation of Allene. Upper-limit k.	EX	300	≤1.81(10)			2
C₃ + CH₃C≡CH → products						
Carbon trimer + 1-Propyne						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-Fluorescence. P(CH ₃ C≡CH) = (0-2.8) torr.	EX	294	(1.98±0.04)(11)			2
82 NEL/HEL C ₃ generated by multiphoton UV-Photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. P(Total) = (5-100) torr. P(CH ₃ C≡CH) = (0-1) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(2.97±0.28)(12)	0	121±35	2
C₃ + CH₂=C=CH₂ → products						
Carbon trimer + 1,2-Propadiene (Allene)						
80 LES/HIC Dye-laser induced fluorescence.	EX	298	2.59(11)			2
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(Allene) = (0-3.71) torr.	EX	294	(5.36±0.36)(10)			2
C₃ + CH₃CH=CH₂ → products						
Carbon trimer + 1-Propene						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(CH ₃ CH=CH ₂) = (0-6.0) torr.	EX	294	(3.03±0.19)(10)			2
82 NEL/HEL C ₃ generated by multiphoton UV-Photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. P(CH ₃ CH=CH ₂) = (0-6.25) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(6.26±0.36)(10)	0	159±21	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
C₃ + CH₃CH₂CH=CH₂ → products						
Carbon trimer + 1-Butene						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(CH ₃ CH ₂ CH=CH ₂) = (0-4.8) torr.	EX	294	(5.52±0.37)(10)			2
82 NEL/HEL C ₃ generated by multiphoton UV-Photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. P(1-Butene) = (0-7) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(7.34±0.30)(10)	0	139±17	2
C₃ + cis-CH₃CH=CHCH₃ → products						
Carbon trimer + 2-Butene, (Z)-						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(cis-2-Butene) = (0-0.98) torr.	EX	294	(2.51±0.08)(11)			2
82 NEL/HEL C ₃ generated by multiphoton UV-Photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. P(cis-2-Butene) = (0-1) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(1.26±0.06)(11)	0	-201±19	2
C₃ + (CH₃)₂C=CH₂ → products						
Carbon trimer + 1-Propene, 2-methyl-						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(Isobutene) < 0.082 torr.	EX	294	(2.91±0.11)(12)			2
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. P(2-Methyl-1-propene) = (0-0.08) torr. P(Benzene) = (1-2) mtorr. P(Total) = (5-100) torr.	EX	295-610	(2.53±0.10)(11)	0	-759±15	2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
C₃ + CH₃CH₂CH₂CH₃ → products						
Carbon trimer + Butane						
82 NEL/HEL	EX	295-610	≤1.20(8)			2
C ₃ generated by Multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. Upper-limit k. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr. P(Butane) = 90 torr.						
C₃ + CH₃CH₂CH₂C≡CH → products						
Carbon trimer + 1-Pentyne						
81 NEL/PAS	EX	294	(3.37±0.19)(11)			2
C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser induced Fluorescence. P(1-Pentyne) = (0-0.48) torr.						
C₃ + CH₃CH=C=CHCH₃ → products						
Carbon trimer + 2,3-Pentadiene						
81 NEL/PAS	EX	294	(6.45±0.54)(11)			2
C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. 2,3-Pentadiene form unspecified (cis, or trans). P(2,3-Pentadiene) = (0-0.4) torr.						
C₃ + (CH₃)₂C=CHCH₃ → products						
Carbon trimer + 2-Butene, 2-methyl-						
81 NEL/PAS	EX	294	(8.97±0.60)(12)			2
C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(2-Methylbut-2-ene) = (0-0.044) torr.						
82 NEL/HEL	EX	295-610	(3.35±0.27)(11)	0	-1014±34	2
C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced Fluorescence. P(2-Methyl-2-Butene) = 90 torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.						
C₃ + CH₃CH₂CH₂C≡CCH₃ → products						
Carbon trimer + 2-Hexyne						
81 NEL/PAS	EX	294	(4.01±0.18)(12)			2
C ₃ generated by multiphoton UV excimer laser Photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(2-Hexyne) = (0-0.1) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. P(2-Hexyne) = (0-0.07) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(6.50±0.05)(11)	0	-695±25	2
C₃ + (CH₃)₂C=C(CH₃)₂ → products						
Carbon trimer + 2-Butene, 2,3-dimethyl-						
82 NEL/HEL C ₃ generated by multiphoton UV-photolysis of C ₆ H ₆ at 249 nm. Laser-induced fluorescence. P(2,3-Dimethyl-2-butene) = (0-0.08) torr. P(Total) = (5-100) torr. P(C ₆ H ₆) = (1-2) mtorr.	EX	295-610	(1.26±0.11)(12)	0	-917±33	2
C₃ + (CH₃)₂C=C=C(CH₃)₂ → products						
Carbon trimer + 2,3-Pentadiene, 2,4-dimethyl-						
81 NEL/PAS C ₃ generated by multiphoton UV excimer laser photolysis of C ₆ H ₆ . Laser-induced Fluorescence. P(2,4-Dimethylpenta-2,3-diene) = (0-0.07) torr.	EX	294	(3.15±0.94)(12)			2
CH₃C≡CD → CH₂=C=CHD (a)						
→ CH₂DC=CH (b)						
1-Propyne-d						
80 HOP/FRI ¹⁾ k _a /k _b . Best data-fit.	RL	853-1033	2.86(-1)			1/1
80 HOP/FRI ¹⁾ k _a + k _b .	EX	853-1033	1.26(11)	0	28334±604	1 2.0
¹⁾ CH ₃ C≡CD pyrolysis in a flow-reactor. P(N ₂) = 760 torr.						
CH₂DC=CH → CH₃C≡CD (a)						
→ CH₂=C=CHD (b)						
1-Propyne-3-d						
80 HOP/FRI ¹⁾ k _a /k _{ref} .	RL	853-1033	3.33(-1)			1/1
80 HOP/FRI ¹⁾ k _b /k _{ref} .	RL	853-1033	2.50(-1)			1/1
¹⁾ CH ₃ C≡CD pyrolysis in a flow-reactor. P(N ₂) = 760 torr. Best data-fit. k _{ref} : CH ₃ C≡CD → CH ₂ DC=CH.						

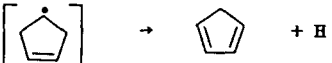
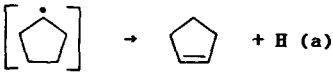
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{C}=\text{CH}_2 (+ \text{M}) \rightarrow \text{CH}_3\text{C}=\text{CH} (+ \text{M})$ (a)						
$\rightarrow \triangle (+ \text{M})$ (b)						
1,2-Propadiene (Allene)						
75 BRA/WES k_a . M = Ar. Limiting high-pressure k.	EX	1440-1700	3.02(14)	0	46670±1925	1 3.63
75 LIF/FRE2 k_a . M = Ar.	EX	1030-1220	1.48(13)	0	30398±1560	1 3.98
78 SIM/MEL k_a . Allene isomerization. Single-pulse shock-tube. M = Ar. P(Total) = 2 atm.	EX	1156-1172	(1.78±0.11)(1)	0	0	1
78 BAI/WAL k_b . Allene cyclization. Pyrolysis in a static system. P(Total) ~ 413 torr.	EX	466-516	1.12(13)	0	32056	1
$\text{CH}_2=\text{C}=\text{CHD} \rightarrow \text{CH}_3\text{C}=\text{CD}$ (a)						
$\rightarrow \text{CH}_2\text{DC}=\text{CH}$ (b)						
1,2-Propadiene-1-d						
80 HOP/PRI 1) k_a/k_{ref} .	RL	853-1033	2.46(-1)	0	0	1/1
80 HOP/PRI 1) k_b/k_{ref} .	RL	853-1033	6.47(-1)	0	0	1/1
1) Pyrolysis in a flow-reactor. Best data-fit. k_{ref} : $\text{CH}_3\text{C}=\text{CD} \rightarrow \text{CH}_2\text{DC}=\text{CH}$. P(N ₂) = 760 torr.						
$\triangle \rightarrow \text{CH}_3\text{C}=\text{CH}$ (a)						
$\rightarrow \text{CH}_2=\text{C}=\text{CH}_2$ (b)						
Cyclopropene						
78 BAI/WAL 2) k_a .	EX	466-516	1.23(13)	0	18776±49	1 1.09
78 BAI/WAL 2) k_a . Limiting high-pressure k. Adjusted value on the basis of theory.	EX	466-516	1.78(13)	0	18861	1
78 BAI/WAL 2) k_b .	EX	466-516	1.78(13)	0	21810	1
2) Pyrolysis in a static system. P(Total) 413 torr.						
$\text{CH}_3\text{CH}=\text{CH}^\dagger \rightarrow \text{CH}_2\text{CH}=\text{CH}_2^\dagger$						
1-Propenyl						
74 IBU/MUR 1)	EX	402	4.04(7)			1
74 IBU/MUR 1)	EX	453	8.38(7)			1
1) $\text{CH}_3\text{CH}=\text{CH}^\dagger$ formed by $\text{CH}_3 + \text{CH}=\text{CH}$.						

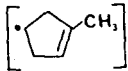
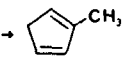
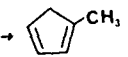
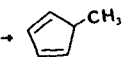

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CHCH}_2^\dagger \rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{H}$						
2-Propenyl (Allyl)						
78 WIE/COL ¹⁾ At 7.1 eV.	EX	298	(5.1±0.3)(6)			1
78 WIE/COL ¹⁾ At 7.6 eV.	EX	298	(1.28±0.07)(7)			1
¹⁾ Photolysis. Static system. Gas-chromatography. $\text{CH}_2=\text{CHCH}_2^\dagger$ formed in photolysis of 1-Pentene by $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^{**} \rightarrow \text{CH}_2=\text{CHCH}_2^\dagger + \text{CH}_3\text{CH}_2$						
$\text{CD}_2=\text{CDCD}_2^\dagger \rightarrow \text{CD}_2=\text{C}=\text{CD}_2 + \text{D}$						
2-Propenyl-1,1,2,3,3-d ₅ (Allyl-d ₅)						
78 WIE/COL ¹⁾ At 7.1 eV.	EX	298	(3.4±0.3)(6)			1
78 WIE/COL ¹⁾ At 7.6 eV.	EX	298	(7.5±0.5)(6)			1
¹⁾ Photolysis. Static system. Gas-chromatography. $\text{CD}_2=\text{CDCD}_2^\dagger$ formed in photolysis of 1-Pentene-d ₁₀ by $\text{CD}_3\text{CD}_2\text{CD}_2\text{CD}=\text{CD}_2^{**} \rightarrow \text{CD}_2=\text{CDCD}_2^\dagger + \text{CD}_3\text{CD}_2$						
$\text{CH}_2=\text{CHCH}_2 + \text{O}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{O}_2$						
2-Propenyl (Allyl) + Oxygen molecule						
81 RUI/BAY M = He. Photoionization Mass-spectrometry. Flash-Photolysis of 1,5-Hexadiene/O ₂ at 193 nm. with an ArF excimer laser. P(Total) = 2.8 torr. P(1,5-Hexadiene) ~100 mtorr. P(O ₂) = (4.1-27.4) mtorr.	EX	348	(9.51±1.91)(10)			2
$\text{CH}_2=\text{CHCH}_2 + \text{NO} (+ \text{M}) \rightarrow \text{C}_3\text{H}_5\text{NO} (+ \text{M})$						
2-Propenyl (Allyl) + Nitrogen oxide (NO)						
82 TUL/MAC ¹⁾ ³⁾	EX	295	(8.13±0.18)(12)			2
82 TUL/MAC ¹⁾ ³⁾	EX	350	(6.74±0.24)(12)			2
82 TUL/MAC ¹⁾ ³⁾	EX	404	(5.60±0.18)(12)			2
¹⁾ Limiting high-pressure k.						
82 TUL/MAC ²⁾ ³⁾	EX	295	(1.45±0.62)(19)			3
82 TUL/MAC ²⁾ ³⁾	EX	350	(9.07±3.63)(18)			3
82 TUL/MAC ²⁾ ³⁾	EX	404	(5.80±2.18)			3
(The product is probably $\text{CH}_2=\text{CHCH}_2\text{NO}$)						
²⁾ Limiting low-pressure k.						
³⁾ M = Ar. 1,5-Hexadiene/NO/Ar flash-photolysis. P(Total) = (50-500) torr. P(NO) = (20-100) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CHCH}_2 + \text{NO}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{O} + \text{NO}$ (a) $\rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{HONO}$ (b)						
2-Propenyl (Allyl) + Nitrogen oxide (NO_2)						
81 SLA/YAM	EX	300	(2.34±0.48)(13)			2
$k_a + k_b$. Allyl radicals generated by pulsed IR-Multiphoton-induced decomposition of Allyl bromide in a tubular reactor. Photoionization Mass-spectrometry. Detection problems prevented determination of channel (b) products. $[\text{NO}_2]_0 = 3.3 \times 10^{12}$ molec. cm^{-3} . P = 1 torr. $[\text{CH}_2=\text{CHCH}_2]_0 < 1.0 \times 10^{11}$ molec. cm^{-3} .						
$\text{CH}_2=\text{CHCH}_2 + \text{CH}=\text{CH} \rightarrow$ 						
2-Propenyl (Allyl) + Ethyne → [3-Cyclopenten-1-yl]						
→ 1,3-Cyclopentadiene + Hydrogen atom						
81 NOH/SAK ¹⁾	ES	723-783	3.98(14)	0	12509	2
81 NOH/SAK ¹⁾	ES	773	4.37(7)			2
¹⁾ Pyrolysis of Ethanedioic acid di-2-propenyl ester, followed by cycloaddition in a flow-reactor. Mass-spectrometry. Same data given in 80 NOH/SAK.						
$\text{CH}_2=\text{CHCH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow$ 						
→ $\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_3$ (b)						
2-Propenyl (Allyl) + Ethene → [Cyclopentyl]						
→ Cyclopentene + Hydrogen atom (a)						
→ 1-Pentene (b)						
81 NOH/SAK ¹⁾	ES	723-783	5.89(9)	0	5774	2
k_a .						
81 NOH/SAK ¹⁾	ES	773	3.31(6)			2
k_a .						
81 NOH/SAK ¹⁾	ES	723-783	1.26(11)	0	8396	2
k_b .						
81 NOH/SAK ¹⁾	ES	773	2.40(6)			2
k_b . For channel (b), the intermediate (Cyclopentyl) abstracts a H atom from any RH to form 1-Pentene.						
¹⁾ Pyrolysis of Ethanedioic acid di-2-propenyl ester followed by cycloaddition in a flow-reactor. Mass-spectrometry. Same data in given 80 NOH/SAK.						


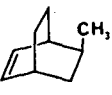
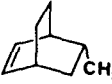
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{CHCH}_2 + \text{CH}\equiv\text{CCH}_3 \rightarrow$ 						
 + H (a)						
 + H (b)						
 + H (c)						
 + CH ₄ (d)						
→ CH ₂ =CHCH ₂ CH=CHCH ₃ (e)						
→ CH ₂ =CHCH ₂ C(CH ₃)=CH ₂ (f)						
2-Propenyl (Allyl) + 1-Propyne						
→ [3-Cyclopenten-1-yl, 3-methyl-]						
→ 1,3-Cyclopentadiene, 2-methyl- + H atom (a)						
→ 1,3-Cyclopentadiene, 1-methyl- + H atom (b)						
→ 1,3-Cyclopentadiene, 5-methyl- + H atom (c)						
→ 1,3-Cyclopentadiene + Methane (d)						
→ 1,4-Hexadiene (e)						
→ 1,4-Pentadiene, 2-methyl- (f)						
81 NOH/SAK ¹) ⁶)	ES	723-783	7.94(13)	0	12269	2
81 NOH/SAK ¹) ⁶)	ES	773	9.33(6)			2
¹) k _a .						
81 NOH/SAK ²) ⁶)	ES	723-783	1.26(14)	0	12870	2
81 NOH/SAK ²) ⁶)	ES	773	7.76(6)			2
²) k _b .						
81 NOH/SAK ³) ⁶)	ES	723-783	2.00(14)	0	14073	2
81 NOH/SAK ³) ⁶)	ES	773	2.24(6)			2
³) k _c .						
81 NOH/SAK ⁴) ⁶)	ES	723-783	2.5(13)	0	12028	2
81 NOH/SAK ⁴) ⁶)	ES	773	4.07(6)			2
The intermediate abstracts a H atom from any RH to form 1,3-Cyclopentadiene and Methane.						
⁴) k _d .						
81 NOH/SAK ⁵) ⁶)	ES	723-783	7.94(11)	0	9659	2
81 NOH/SAK ⁵) ⁶)	ES	773	3.24(6)			2
The intermediate abstracts a H atom from any RH to form 1,4-Hexadiene.						
⁵) k _e .						


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref))	n	B, B-B(ref)	k, A k err. units factor
81 NOH/SAK ⁶⁾ k _f . The intermediate abstracts a H atom from any RH to form 2-Methyl-1,4-pentadiene.	ES	773	1.48(6)			2
⁶⁾ Pyrolysis of Ethanedioic acid di-2-propenyl ester, followed by cycloaddition in a flow-reactor. Gas-chromatography. Mass-spectrometry. The intermediate is 3-Methylcyclopent-3-en-1-yl radical.						
$\text{CH}_2=\text{CHCH}_2 + \text{CH}_2=\text{CHCH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2$						
2-Propenyl (Allyl)						
79 ROS/KIN ¹⁾	EX	625	(6.5±1.0)(12)			2
79 ROS/KIN ¹⁾	EX	880	(1.9±0.8)(12)			2
Average of 7 k's determined at various temperatures within the 844-922 K range.						
¹⁾ VLP-pyrolysis.						
82 TUL/MAC	EX	293-571	(1.02±0.02)(13)	0	-132±12	2
2-Propenyl generated by 1,5-Hexadiene Flash-photolysis in Ar. P(1,5-Hexadiene) = (0.04-1.0) torr. P(Ar) = (0-250) torr.						
$\text{CH}_3\text{CH}=\text{CH}_2 (+ \text{M}) \rightarrow \text{CH}_3 + \text{CH}_2=\text{CH} (+ \text{M}) (\text{a})$ → any other products (b)						
1-Propene						
74 BAK/NOV	EX	973-1123	2.3(14)	0	37141±1510	1
k _{overall} .						
75 BUR	EX	1160-1700	1.0(13)	0	37242±503	2 3.16
k _a . M = Ar. Concentration-dependent k, with Arrhenius expression = k/[Ar].						
82 KIE/ALA ¹⁾	EX	1650-2300	7.71(36)	-15.7	60393	2
The preexponential factor expressed as: A(T/298) ^{-15.7} .						
82 KIE/ALA ¹⁾	DE	2000	6.20(10)			2
¹⁾ k _a . M = Kr, or 1-Propene. Pyrolysis of 1-Propene behind incident shock-waves. Laser-schlieren. k derived from a simulation-assisted extrapolation-measured density gradient to the presumed instant of shock-heating. [M] = (0.6-1.3) × 10 ¹⁸ molec.cm ⁻³ . P = (2.8-10.3) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}=\text{CH}_2 \dagger \rightarrow \text{H} + \text{CH}_2=\text{CHCH}_2$							
1-Propene							
80 IBU/TAK Decomposition of chemically activated 1-Propene, generated by combination of CH_3 with $\text{CH}_2=\text{CH}$. CH_3 generated by the Hg-photosensitized decomposition of CH_4 . $\text{CH}_2=\text{CH}$ generated by combination of H with $\text{CH}=\text{CH}$.	EX	288	(5.04±0.11)(7)			1	
$\text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CH}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (b) $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}=\text{CH}_2$ (c)							
1-Propene							
73 SIM/BAC k_a .	EX	743-803	2.51(13)	0	21892	2	
78 RIC/BAC $k_b = k_c$. Pyrolysis in a static system. P(olefin) = (33-300) torr.	EX	682-754	3.55(9)	0	18621±503	2	2.0
$\text{CH}_3\text{CH}=\text{CH}_2 + $  $\rightarrow $  (a)							
$\rightarrow $  (b)							
1-Propene + 1,3-Cyclohexadiene \rightarrow \rightarrow Bicyclo[2.2.2]oct-2-ene, 5-methyl- (1 α ,4 α ,5 α)- (Exo form) (a) \rightarrow Bicyclo[2.2.2]oct-2-ene, 5-methyl-, (1 α ,4 α ,5 β)- (Endo form) (b)							
74 DEB/HUY ¹⁾ k_a .	EX	512-638	4.57(9)	0	15143±40	2	1.07
74 DEB/HUY ¹⁾ k_b .	EX	512-638	5.50(8)	0	13120±40	2	1.07
¹⁾ Addition of Propene to 1,3-Cyclohexadiene in a cylindrical Pyrex reaction vessel. Gas-chromatography. Mass-spectrometry. P = (70-640) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\triangle \rightarrow \text{CH}_2\text{CH}=\text{CH}_3$ (a)						
\rightarrow any other products (b)						
Cyclopropane						
73 DOR/CRO k_a . M = Ar. Cyclopropane thermal isomerization behind reflected shock-waves.	EX	1158-1323	5.0(9)	0	16104	1 3.0
78 TSA2 ¹⁾ k_a . P = 1.7 Atm.	EX	1000-1200	1.26(14)	0	31100±200	1 1.26
78 TSA2 ¹⁾ k_a . P = 5.0 Atm.	EX	1000-1200	2.0(14)	0	31100±100	1 1.26
¹⁾ Cyclopropane Thermolysis in a single-pulse shock-tube in Ar, in presence of Cyclohexane and Toluene. k's determined relative to the reaction:						
						
[Cyclopropane] = 0.01%. [Cyclohexene] = 0.01%. P(Ar) ~ (1.7-7) atm. [Toluene] = 1%.						
71 DOR/MCG k_a . M = He + Ar. Cyclopropane isomerization to 1-Propene behind reflected shock-waves. Limiting high-pressure k. [Cyclopropane] = (0.1-1.0)% P ₀ = (103-259) torr.	EX	935-1397	3.16(14)	0	32763±403	1 1.38
73 JEF/DAS k_a . M = Ar. Cyclopropane thermal isomerization in a single-pulse shock-tube. Measurement relative to the Cyclohexane decomposition. Gas-chromatography.	RN	980-1040	1.82(15)	0	33669	1
73 JEF/LEW k_a . M = Ar. Cyclopropane Thermal isomerization behind reflected shock-waves, in a single-pulse shock-tube. Limiting high-pressure k. [Cyclopropane] = (0.25-10)% P(Total) = (0.5-7.0) atm.	EX	970-1265	1.58(15)	0	32713	1
74 BAR/COC ²⁾	EX	950	4.43			1
74 BAR/COC ²⁾	EX	1052	1.35(2)			1
74 BAR/COC ²⁾	EX	1096	8.73(2)			1
74 BAR/COC ²⁾	EX	1302	2.16(3)			1
74 BAR/COC ²⁾	EX	1452	5.96(3)			1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 BAR/COC ²⁾	EX 1653		2.34(4)			1
²⁾ k_a . M = He + Ar. Cyclopropane thermal isomerization behind reflected shock-waves in a single-pulse shock-tube. Limiting high-pressure k. Other rate constants at various temperatures within the 950-1653 K range are tabulated. The Arrhenius plot shows a pronounced curvature in the vicinity of 1080 K. [Cyclopropane] = (0.2-1.0)%.						
71 BRA/FRE ³⁾	EX 1060-1300		7.94(11)	0	27665	1
71 BRA/FRE ³⁾	EX 1350-1800		5.62(4)	0	5834	1
³⁾ $k_{overall}$. M = Ar. Shock-tube pyrolysis. P(Total) = 500 torr.						



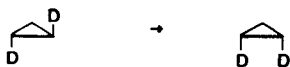
(Racemic mixture)

Cyclopropane-1,2-d₂, (1S-trans)-
 → Cyclopropane-1,2-d₂, cis- (a)
 → Cyclopropane-1,2-d₂, trans-(±)- (racemic) (b)

76 BER/PED ¹⁾ EX 696 (6.75±0.14)(-5) 1
 k_a . Thermal trans-cis isomerization.

76 BER/PED ¹⁾ EX 696 (6.33±0.14)(-5) 1
 k_b . Thermal racemization.

¹⁾ trans-(+)-Cyclopropane-1,2-d₂ thermal stereomutation. Gas-chromatography.
 Supersedes 75 BER/PED.
 P = 631 torr.




Cyclopropane-1,2-d₂, (1R-trans)-
 → Cyclopropane-1,2-d₂, cis-

76 BER/PED EX 696 (6.75±0.14)(-5) 1

Thermal trans-cis isomerization of optically active trans-(-)-Cyclopropane-1,2-d₂ in a reaction vessel. Gas-chromatography.
 Supersedes 75 BER/PED.
 P = 631 torr.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CH₂CH₂ (+ M) → CH₃ + CH₂=CH₂ (+ M)							
Propyl							
71 PAP/LAI Limiting high-pressure k. M = CH ₃ CH ₂ CH ₃	EX	525-623	2.5(14)	0	16407±252	1	
75 CAM/MAR	EX	676-813	1.26(12)	0	16359±962	1	3.16
80 GAW/MAK ¹⁾ At 228.8 nm.	EX	298	2.9(10)			1	
80 GAW/MAK ¹⁾ At 253.7 nm.	EX	298	7.0(9)			1	
¹⁾ H ₂ S irradiation with UV-light. Reaction of hot H atoms with Propene in a conventional vacuum system. Best data fit. P = (0.4-760) torr.							
71 PAP/LAI Limiting low-pressure k. M = CH ₃ CH ₂ CH ₃	EX	525-623	2.5(7)	0	8556±252	2	
CH₃CH₂CH₂ + O₂ → CH₃CH=CH₂ + HO₂ (a)							
→ CH ₃ CH ₂ CHO + OH (b)							
→  + OH (c)							
→ CH ₃ CH ₂ CH ₂ O ₂ (d)							
Propyl + Oxygen molecule							
71 BAK/BAL ¹⁾ Least-squares treatment.	RL	753	(1.41±0.23)(6)				2/1
71 BAK/BAL ¹⁾ Computer treatment.	RL	753	(1.25±0.20)(6)				2/1
¹⁾ k _a /k _{ref} . k _{ref} : CH ₃ CH ₂ CH ₂ → CH ₃ + CH ₂ =CH ₂							
71 BAK/BAL k _a .	ES	753	3.8(10)				2
71 BAK/BAL k _b .	ES	753	1.1(8)				2
71 BAK/BAL k _c .	ES	753	3.1(9)				2
82 RUI k _d . M = N ₂ . Photoionization mass-spectrometry. k increases with the pressure. Near high-pressure limiting k. P(Total) = 4 torr.	EX	298	(3.43±0.10)(13)				2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
CH₃CH₂CH₂ + O₃ → products						
Propyl + Ozone						
82 FAL Photoionization mass-spectrometry. Propyl formed by photodissociation of CH ₃ CH ₂ CH ₂ NO ₂ . P = 2 torr.	EX	298	(1.47±0.29)(13)			2
CH₃CH₂CH₂ + HCHO → CH₃CH₂CH₃ + CHO (a) → CH₃CH₂CH₂CH₂O (b)						
Propyl + Formaldehyde						
80 KNO/NAC ¹⁾ k _a .	RN	333-363	1.0(11)	0	3921±253	2 2.0
80 KNO/NAC ¹⁾ k _b .	RN	333-363	7.94(10)	0	3367±253	2 3.16
¹⁾ Azopropane/Formaldehyde photolysis. Mass-spectrometry.						
CH₃CH₂CH₂ + CH≡CH → cis-CH₃CH₂CH₂CH=CH[†] (a) → trans-CH₃CH₂CH₂CH=CH[†] (b)						
Propyl + Ethyne						
72 WAT/OLS k _a + k _b . Azo-n-propane photolysis. P = (90-480) torr.	ES	343-405	1.15(12)	0	4529	2
CH₃CH₂CH₂ + CH₂=CH₂ → CH₃CH₂CH₂CH₂CH₂[†]						
Propyl + Ethene						
71 WAT/LAW Azo-n-propane Photolysis. k determined relative to the reaction: CH ₃ CH ₂ CH ₂ + CH ₃ CH ₂ CH ₂ · → CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ CH ₃	ES	330-373	1.41(11)	0	3724	2
CH₃CH₂CH₂ + CH₃CH₂CH₂ → CH₃CH=CH₂ + CH₃CH₂CH₃ (a) → CH₃CH₂CH₂CH₂CH₂CH₃ (b)						
Propyl						
71 FAL/SUN k _a /k _b .	RL	298	1.5(-1)			2/2
81 ADA/BAS1 ¹⁾ k _a .	EX	298	(1.9±0.2)(12)			2
81 ADA/BAS1 ¹⁾ k _b .	EX	298	(1.0±0.1)(12)			2
¹⁾ Azo-n-propane Flash-photolysis. Kinetic Spectroscopy.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{CH}_2 + (\text{CH}_3)_2\text{CH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_3$ (a) $\quad \quad \quad \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3$ (b)						
Propyl + Ethyl, 1-Methyl- (i-Propyl)						
71 FAL/SUN k_a/k_b .	RL	298	4.1(-1)			2/2
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CO}$ (a) $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CHCHO}$ (b) $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CHCH}_2\text{CHO}$ (c)						
Propyl + Butanal						
79 FOE/BER ¹⁾ k_a .	DE	273-529	1.0(11)	0	3322±252	2 2.0
79 FOE/BER ¹⁾ k_b .	DE	273-529	3.98(10)	0	4328±352	2 3.16
79 FOE/BER ¹⁾ k_c .	DE	426-529	3.98(10)	0	5184	2
¹⁾ Butanal photolysis. Rate constants determined relative to the reaction: $\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ on the basis of a suggested reaction scheme.						
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ (b) $\quad \quad \quad \rightarrow \text{CH}_3(\text{CH}_2)_6\text{CH}_3$ (c)						
Propyl + Pentyl						
71 WAT/LAW ¹⁾ $(k_a + k_b + k_c)/k_c$. Estimated ratio.	RL	330	1.14			2/2
71 WAT/LAW ¹⁾ k_b/k_c .	RL	330	5.6(-2)			2/2
¹⁾ Azo-n-propane Photolysis.						
$\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3$ $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_3$ (b) $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{cis-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$ (c) $\quad \quad \quad \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{trans-CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3$ (d) $\quad \quad \quad \rightarrow (\text{CH}_3\text{CH}_2\text{CH}_2)_2\text{CH}(\text{CH}_3)$ (e)						
Propyl + Butyl, 1-methyl-						
71 WAT/LAW $(k_a + k_b + k_c + k_d + k_e)/k_e$. Azo-n-propane Photolysis. Estimated ratio.	RL	330	1.41			2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CH} \rightarrow \text{H} + \text{CH}_3\text{CH}=\text{CH}_2$ (a)						
$\rightarrow \text{CH}_3 + \text{CH}_2=\text{CH}_2$ (b)						
Ethyl, 1-methyl- (i-Propyl)						
71 PAP/LAI k_a . Limiting high-pressure k. M = $\text{CH}_3\text{CH}_2\text{CH}_3$.	EX	525-623	2.0(14)	0	19480	1
75 CAM/MAR k_a .	EX	676-813	2.51(13)	0	20569±1202	1 5.01
75 BUL/MAR k_b/k_a . Static system pyrolysis. Average ratio.	RL	667-770	4.0(-2)	0	0	1/1
$(\text{CH}_3)_2\text{CH}^\ddagger \rightarrow \text{H} + \text{CH}_3\text{CH}=\text{CH}_2$ (a)						
$\rightarrow \text{CH}_3 + \text{CH}_2=\text{CH}_2$ (b)						
Ethyl, 1-methyl- (-Propyl)						
72 ARI/STE ¹⁾ k_a .	ES	²⁾	1.0(14)	0	20634	1
72 ARI/STE ¹⁾ k_b .	ES	²⁾	1.0(14)	0	23150	1
1) $(\text{CH}_3)_2\text{CH}^\ddagger$ formed by Photolysis of Azoisopropane.						
2) Arrhenius expression determined from a pressure-wavelength data-fit to the RRKM theory.						
$(\text{CH}_3)_2\text{CH} + \text{O}_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{HO}_2$ (a)						
$\rightarrow (\text{CH}_3)_2\text{CHO}_2$ (b)						
Ethyl, 1-methyl- (i-Propyl) + Oxygen molecule						
76 BAL/CLE ¹⁾ k_{ref} : $(\text{CH}_3)_3\text{CH} + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{H}$	RL	713	(3.06±0.25)(3)			2/2
76 BAL/CLE ¹⁾ k_{ref} : $(\text{CH}_3)_3\text{CH} + \text{D}_2 \rightarrow \text{CH}_3\text{CHDCH}_3 + \text{D}$	RL	713	(7.68±0.30)(3)			2/2
1) k_a/k_{ref} .						
82 RUI k_b . M = He. Photoionization Mass-spectrometry. Near high-pressure limiting k. k is P-independent. P(Total) = 1 torr.	EX	298	(7.83±1.20)(12)			2
$(\text{CH}_3)_2\text{CH} + \text{O}_3 \rightarrow \text{products}$						
Ethyl, 1-methyl- (i-Propyl) + Ozone						
82 PAL Photoionization mass-spectrometry. $(\text{CH}_4)_2\text{CH}$ formed by photodissociation of $(\text{CH}_3)_2\text{CHNO}_2$. P = 2 torr.	EX	298	(2.80±0.32)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_2\text{CH} + \text{H}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{H}$							
Ethyl, 1-methyl- (i-Propyl) + Hydrogen molecule							
76 BAL/CLE	RL	713	(2.51±0.20)				2/2
$k_{\text{ref}}:$							
$(\text{CH}_3)_2\text{CH} + \text{D}_2 \rightarrow \text{CH}_3\text{CHDCH}_3 + \text{D}$							
$(\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_3\text{CH}_2$							
Ethyl, 1-methyl- (i-Propyl) + Ethane							
74 SZI/MAR	RN	496-548	2.511(10)	0	6392±403	2	2.51
76 SZI/MAR	RN	496-548	1.0(11)	0	6495±361	2	2.51
Azoisopropane sensitized pyrolysis of Ethane in a static system. k determined relative to the reaction: $(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ P = (38-230) torr.							
$(\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_2=\text{CCH}_2$							
Ethyl, 1-methyl (i-Propyl) + 1-Propene							
76 SZI/MAR	RN	496-548	5.01(9)	0	3850±850	2	5.01
Azoisopropane sensitized pyrolysis of Ethane in a static system. k determined relative to the reaction: $(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ P = (38-230) torr.							
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_3$ (a)							
$\rightarrow (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ (b)							
Ethyl, 1-methyl- (i-Propyl)							
71 FAL/SUN ¹⁾	RL	298	6.9(-1)				2/2
72 ARI/STE ¹⁾	RL	295	(5.7±0.5)(-1)				2/2
Azoisopropane Photolysis.							
74 GOL/PIS ¹⁾	RL	683	(1.0±0.5)				2/2
74 GOL/PIS ¹⁾	RL	808	(1.5±0.5)				2/2
76 PAR/QUI ¹⁾	RL	298	(6.5±0.5)(-1)				2/2
77 MCK/TUR ¹⁾	RL	518	5.2(-1)				2/2
Azoisopropane thermolysis.							
77 MCK/TUR ¹⁾	RL	573	4.9(-1)				2/2
Azoisopropane thermolysis.							
79 KIR/PAR ¹⁾	RL	302	(6.0±0.1)(-1)				2/2
Photolysis of trans-2,2'-Azopropene.							
Gas-chromatography. Mass-spectrometry.							
79 SZI ¹⁾	RL	494-546	(7.6±1.6)(-1)				2/2
Azoisopropane pyrolysis in a static system.							
Average ratio:							
¹⁾ k_a/k_b .							




4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 ARR/KIR k_a . Molecular Modulation Spectrometer technique.	EX	301-424	(3.01±0.60)(12)	0	-25±313	2	
81 ADA/BAS1 k_a . Flash-photolysis of Azoisopropane. Kinetic spectroscopy.	EX	298	(5.0±1.2)(12)			2	
82 DEM/LES $k_a + k_b$. Flash-photolysis. Laser-resonance-absorption. (CH ₃) ₂ CH generated by flashing NH ₃ in presence of 1-Propene. Best data-fit.	ES	298	6.0(12)			2	
72 HIA/BEN1 ¹⁾	ES	415	3.98(11)			2	12.6
74 GOL/PIS ¹⁾	RN	683-808	3.16(12)	0	0	2	1.58
76 PAR/QUI ¹⁾	RN	298	(5.0±1.2)(12)			2	
78 ARR/KIR ¹⁾ Molecular Modulation Spectrometer technique.	EX	301-424	(8.43±1.69)(12)	0	161±313	2	
81 ADA/BAS1 ¹⁾ Flash-photolysis of Azoisopropane.	EX	298	(7.7±1.6)(12)			2	
¹⁾ k_b .							
(CH ₃) ₂ CH + (CH ₃) ₂ CHCHO → CH ₃ CH ₂ CH ₃ + (CH ₃) ₂ CHCO (a) → CH ₃ CH ₂ CH ₃ + (CH ₃) ₂ CCHO (b)							
Ethyl, 1-methyl- (i-Propyl) + Propanal, 2-methyl-							
76 BAL/CLE ($k_a + k_b$)/ k_{ref} . k_{ref} : (CH ₃) ₂ CH + O ₂ → CH ₃ CH=CH ₂ + HO ₂	RL	713	3.2(-3)			2/2	1.1
(CH ₃) ₂ CH + (CH ₃) ₄ C → CH ₃ CH ₂ CH ₃ + (CH ₃) ₃ CCH ₂							
Ethyl, 1-methyl- (i-Propyl) + Propane, 2,2-dimethyl- (Neopentane)							
79 SZI/MAR Neopentane pyrolysis in presence of Azo- isopropane. P(Total) = (15-300) torr.	EX	512-571	3.16(10)	0	6616±601	2	6.31
(CH ₃) ₂ CH + (CH ₃) ₂ CHCH(CH ₃) ₂ → CH ₃ CH ₂ CH ₃ + (CH ₃) ₂ CHCH(CH ₃)CH ₂ (a) → CH ₃ CH ₂ CH ₃ + (CH ₃) ₂ CHC(CH ₃) ₂ (b)							
Ethyl, 1-methyl- (i-Propyl) + Butane, 2,3-dimethyl-							
75 BUL/MAR ¹⁾ ($k_a + k_b$)/ k_{ref} . k_{ref} : (CH ₃) ₂ CH → H + CH ₃ CH=CH ₂	RL	667-770	6.31(-1)	0	-9863	2/1	
75 BUL/MAR ¹⁾ $k_a + k_b$.	ES	667-770	1.58(13)	0	10710	2	
¹⁾ Static system pyrolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{CH}_2\text{CH}(\text{CH}_3)\text{N}=\text{NCH}(\text{CH}_3)_2$							
Ethyl, 1-methyl- (i-Propyl) + Diazene, bis(1-methylethyl)- (Azoisopropane)							
79 SZI Azoisopropane pyrolysis in a static system.	EX	494-546	5.01(9)	0	3248±241	2	1.58
$\text{CH}_3\text{CH}_2\text{CH}_3 (+\text{M}) \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2 (+\text{M})$ (a) $\rightarrow \text{any other products } (+\text{M})$ (b)							
Propane							
79 FRA/ROG2 k _a . M = Ar. Pyrolysis in a wall-less reactor. Average k at the mean experimental T. Other k values within (967-1051) K T-range also given. Approximate fitted values. P(Ar) = 600 torr.	EX	1008	(3.0±1.5)(-3)			1	
81 CHI/SKI1 ¹⁾ k _a . Experimental k.	EX	1200-1450	6.7(16)	0	45395	1	
81 CHI/SKI1 ¹⁾ k _a . Recommended k.	SE	1200-1450	2.5(16)	0	44036	1	2.0
1) Pyrolysis behind reflected shock-waves. Resonance-absorption spectroscopy. Same data given in 79 CHI/SKI. P (Total) = (2-3) atm.							
81 JUS/SCA k _a . Pyrolysis in a jet-stirred tank-reactor. Gas-chromatography. P(Propane) ~20 torr.	EX	873-1053	≈4.47(16)	0	≈42627	1	
82 ALA k _a . Pyrolysis behind incident shock-waves. Laser-schlieren. Limiting high-pressure k. P = (150-550) torr.	EX	1400-1800	7.74(11)	0	28048	1	
72 ILL/SZA ²⁾	EX	910-1075	6.37(13)	0	31807	1	1.1
74 BAK/NOV ²⁾	EX	973-1123	3.5(12)	0	28737±1007	1	
78 VER/BEL ²⁾ Pyrolysis in a flow-reactor. Average ratio. k _{ref} : $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}$.	RL	873-1103	(6.35±1.05)(-1)			1/1	
79 BRA ²⁾ Pyrolysis in a single-pulse shock-tube.	EX	1210-1680	1.98(8)	0	18885	1	1.38
79 ZYC/BAC ²⁾ Pyrolysis in a tubular reactor. P = 1 atm.	EX	1000-1120	1.7(11)	0	26572±352	1	
81 HAU/SAN ²⁾ Pyrolysis in a flow-reactor.	EX	1110-1235	3.16(12)	0	29517±906	1	2.19
2) k _{overall} .							


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 CHI/SKI k_a . M = Ar. Pyrolysis behind reflected shock-waves. P = (2-3) Atm.	EX	1200-1450	2.6(21)	0	45244	2
82 ALA k_a . Pyrolysis behind incident shock-waves. Limiting low-pressure k. P = (150-550) torr.	EX	1800-2300	2.68(17)	0	28278	2
$\text{CH}_3\text{CH}_2\text{CH}_3^\ddagger \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2$ (a) $\rightarrow \text{CH}_4 + \text{CH}_2=\text{CH}_2$ (b)						
Propane						
71 LEX/MAR1 ¹⁾ k_a . P(Ar) = (4-16) torr.	RL	290	(3.99±0.46)(-8)			1/2
72 GRO/HAS k_a .	EX	298	(4.7±1.2)(8)			1
71 LEX/MAR1 ¹⁾ k_b . P(Ar) = (4-16) torr.	RL	290	(3.22±0.28)(-8)			1/2
71 LEX/MAR2 ¹⁾ k_b . P(Ar) = (4-12) torr.	RL	290	(3.28±0.41)(-8)			1/2
¹⁾ M = Ar. Discharge flow. $\text{CH}_3\text{CH}_2\text{CH}_3^\ddagger$ formed by H + (CH ₃) ₂ CH. k_{ref} : $\text{CH}_3\text{CH}_2\text{CH}_3^\ddagger + \text{M} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_3 + \text{M}$.						
$\text{CD}_3\text{CD}_2\text{CD}_3 \rightarrow \text{CD}_3 + \text{CD}_3\text{CD}_2$						
Propane-d ₈						
81 CHI/SKI1 ¹⁾	EX	1200-1450	6.7(16)	0	45395	1
81 CHI/SKI1 ¹⁾ Recommended k.	SE	1200-1450	2.5(16)	0	44036	1 2.0
¹⁾ Pyrolysis behind reflected shock-waves. Resonance-absorption spectroscopy. Same data given in 79 CHI/SKI. P(Total) = (2-3) atm.						
$\text{CH}_2=\text{CHCHO} + $  $ \rightarrow $  $ \text{CHO}$ (a)						
$ \rightarrow $  $ \text{CHO}$ (b)						
2-Propenal (Acrolein) + 1,3-Cyclohexadiene \rightarrow Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, (1 α , 2 α , 4 α)- (Exo form) (a) \rightarrow Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, (1 α , 2 β , 4 α)- (Endo form) (b)						
76 HUY/PAT ¹⁾ k_a .	EX	486-871	3.24(5)	0	10382±25	2 1.05

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 HUY/PAT ¹⁾ k _b .	EX	486-871	4.47(5)	0	9799±25	2	1.05
¹⁾ Diels-Alder addition of Acrolein to 1,3-Cyclohexadiene in a Pyrex reaction vessel. Gas-chromatography. P = (55-240) torr.							
CH₃CH₂CO (+ M) → CH₃CH₂ + CO (+ M)							
Propyl, 1-oxo-							
73 WAT/THO	ES	238-278	5.89(12)	0	7247	1	
76 ERN/SPI	EX	1350-1650	2.7(16)	0	41137±1443	1	
M = Ar. Limiting high-pressure k. Supersedes 75 ERN/SPI.							
CH₃CH₂CO + O₂ → CH₂=CH₂ + CO₂ + OH							
Propyl, 1-oxo- + Oxygen molecule							
79 BAL/LEW1	RL	713	(1.12±0.10)(-1)			2/2	
M = N ₂ . Oxidation in an aged boric-acid-coated vessel. k _{ref} : CH ₃ CH ₂ CO + M → CH ₃ CH ₂ + CO + M							
CH₂=C(CH₂)O₂ → CH₂=CHCH₂ + O₂							
2-Propenyldioxy							
81 RUI/BAY	EX	348	(2.60±0.96)(1)			1	
M = He. Photoionization mass-spectrometry. k ₁ Measured simultaneously with k ₋₁ . Allyl formed by Hexadiene/O ₂ flash-photolysis at 193 nm., with anArF excimer laser. P(1,5-Hexadiene) ~100 mtorr. P(O ₂) = (4.1-27.4) mtorr. P(Total) = 2.8 torr.							
CH₃CH₂CHO + CH₃CH₂C(O)OOH → products							
Propanal + Propaneperoxoic acid							
74 DIX/SKI1	RN	337	1.0			2	
□^O → HCHO + CH₂=CH₂							
Oxetane							
75 HOL/SCO	EX	693-753	5.13(15)	0	31719±422	1	2.04
Pyrolysis in a cylindrical Pyrex vessel. High-vacuum system. Gas-chromatography. NMR, and IR-Spectrometry. P _o = (0.4-117) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow \text{CH}_3\text{CH}_2\text{CHO}$ (a) $\rightarrow (\text{CH}_3)_2\text{CO}$ (b) $\rightarrow \text{CH}_2=\text{CHCH}_2\text{OH}$ (c) $\rightarrow \text{CH}_2=\text{CHOCH}_3$ (d)							
Oxirane, methyl-							
77 FLO 1) k_a . $P_o = 131$ torr.	EX	654-717	2.45(14)	0	29434±289	1	1.51
77 FLO 1) k_b . $P_o = 131$ torr.	EX	654-717	1.51(14)	0	30131±289	1	1.51
77 FLO 1) k_b . Limiting high-pressure k. RRKM calculation.	ES	654-717	1.70(14)	0	30552	1	
77 FLO 1) k_c . $P_o = 131$ torr.	EX	654-717	7.94(12)	0	28760±241	1	1.41
77 FLO k_d . $P_o = 131$ torr.	EX	654-717	3.24(14)	0	29578±373	1	1.70
77 FLO 1) 2) Without added NO.	EX	654-717	4.37(14)	0	29470±156	1	1.26
77 FLO 1) 2) Packed reaction vessel without added NO.	EX	654-717	3.09(14)	0	29145±397	1	1.78
77 FLO 1) 2) With 8.5% NO added.	EX	654-717	4.07(14)	0	29482±229	1	1.38
1) Thermolysis in a static system. Gas-chromatography. Mass-spectrometry. $P = (5-326)$ torr.							
2) $k_a + k_b + k_c + k_d$.							
HC(O)OCH ₂ CH ₃ → products Formic acid ethyl ester (Ethyl formate)							
71 BLA/SAN	EX	830-903	2.19(12)	0	24207±252	1	
CH ₃ C(O ¹⁸)OCH ₃ → CH ₃ COO ¹⁸ CH ₃ Acetic- ¹⁸ O acid ¹⁸ O-methyl ester							
81 CAR/EGS 1)	EX	1253	3.72(2)			1	
81 CAR/EGS 1)	EX	1404	1.78(3)			1	
1) Flash-vacuum thermolysis.							
CH ₃ C(O)OCH ₃ → products Acetic acid methyl ester (Methyl acetate)							
82 BLA/SHR Thermolysis. Apparent k, reflecting the importance of heterogeneous processes in the decomposition. $P(\text{Methyl acetate})_o = (30-70)$ torr.	EX	743-834	2.00(6)	0	17358±780	1	2.63

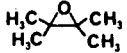
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
<hr/>							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO} \rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{HNO}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}$ (b)							
Propoxy + Nitrogen oxide (NO)							
80 ROS k_a/k_b . Propyl nitrite/ NO_2 photolysis at 366 nm.	RL	298	(1.1±0.1)(-1)				2/2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{HONO}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{ONO}_2$ (b)							
Propoxy + Nitrogen oxide (NO_2)							
80 ROS k_a/k_b . Propyl nitrite photolysis at 366 nm. in presence of NO_2 . Gas-chromatography.	RL	298	(1.1±0.1)(-1)				2/2
75 MEN/GOL k_b . Estimated from thermochemical data and the assumption that $E_a \sim 0$.	DE	300	3.16(12)	0	0		2
77 BAR/BEN2 k_b . VLP-Pyrolysis. RRKM best-fit estimate.	ES	580-800	3.16(12)				2
$(\text{CH}_3)_2\text{CHO} \rightarrow \text{CH}_3\text{CHO} + \text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CO} + \text{H}$ (b)							
Ethoxy, 1-methyl-							
75 BAT/MCC k_a .	ES	393-473	2.51(14)	0	8606		1
79 BAT ¹⁾ k_a .	ES	393-473	3.98(14)	0	8656±503		1 3.16
79 BAT ¹⁾ k_b . Preliminary k.	ES	393-473	2.00(14)	0	10820		1
¹⁾ Static system. Same data given in 77 BAT/MIL1.							
$(\text{CH}_3)_2\text{CHO} + \text{NO} \rightarrow (\text{CH}_3)_2\text{CHONO}$ (a) $\rightarrow (\text{CH}_3)_2\text{CO} + \text{HNO}$ (b) $\rightarrow (\text{CH}_3)_2\text{CHONO}$ (c)							
Ethoxy, 1-methyl- + Nitrogen oxide (NO)							
74 BAT/MIL ¹⁾ k_a .	ES	393-473	2.51(13)	0	0±503		2 2.51
77 BAT/MIL ¹⁾ k_a .	ES	403-433	3.16(13)	0	0±403		2 2.51
74 BAT/MIL ²⁾ k_b .	ES	393-473	3.98(12)	0	0±503		2 3.16
77 BAT/MIL ²⁾ k_b .	ES	503-433	3.16(13)	0	0±503		2 2.51
74 BAT/MIL k_c .	ES	393-473	2.51(13)	0	0±503		2 2.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CHO} + (\text{CH}_3)_2\text{CHOOH} \rightarrow (\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHOH}$ Ethoxy, 1-methyl- + Hydroperoxide, 1-methylethyl- 79 KIR/PAR trans-2,2'-Azopropane photolysis. Mass-spectrometry. $k_{\text{ref}}: (\text{CH}_3)_2\text{CHO} + \text{O}_2 \rightarrow (\text{CH}_3)_2\text{CO} + \text{HO}_2.$	RL	302	(1.66±0.05)(-2)			2/2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{O}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{O}_2$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{CH}_3\text{CH}_2\text{CH}_2\text{O} + \text{O}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{OH} + \text{CH}_3\text{CH}_2\text{CHO} + \text{O}_2$ (b) Propylldioxy 82 ADA/BAS1 $k_a + k_b.$ Azo-n-propane Flash-photolysis in Ar. P(Azo-n-propane) = (4.5-10) torr. P(Pentane) = (0-86) torr. P(O ₂) = (2.2-670) torr. P(Ar) = (0-540) torr. P(N ₂) = (0-720) torr.	EX	298	(2.0±0.2)(8)			2
$(\text{CH}_3)_2\text{CHO}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{NO}_2$ Ethylldioxy, 1-methyl- + Nitrogen oxide (NO) 82 ADA/BAS2 Azoisopropane Flash-photolysis. Kinetic-spectroscopy. k is P-independent in the (55-400) torr. range. P(NO ₂) = (1.1-6.1)×10 ⁻² torr. P(NO) = (1.4-6.1)×10 ⁻² torr. P(Azoisopropane) ~2 torr. P(O ₂) = (5.7-15.5) torr.	EX	298	(2.1±0.2)(12)			2
$(\text{CH}_3)_2\text{CHO}_2 + \text{NO}_2 \rightarrow (\text{CH}_3)_2\text{CHOONO}_2$ Ethylldioxy, 1-methyl- + Nitrogen oxide (NO ₂) 82 ADA/BAS2 Azoisopropane Flash-photolysis. Kinetic spectroscopy. k is P-independent in the (55-400) torr. range. P(NO ₂) = (1.1-6.1)×10 ⁻² torr. P(NO) = (1.4-6.1)×10 ⁻² torr. P(Azoisopropane) ~2 torr. P(O ₂) = (5.7-15.5) torr.	EX	298	(3.4±0.1)(12)			2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHO}_2$							
→ $(\text{CH}_3)_2\text{CHO} + (\text{CH}_3)_2\text{CHO} + \text{O}_2$ (a)							
→ $(\text{CH}_3)_2\text{CHOH} + (\text{CH}_3)_2\text{CO} + \text{O}_2$ (b)							
Ethyldioxy, 1-methyl-							
79 KIR/PAR	EX	302	(2.99±0.20)(8)				2
k_a . trans-2,2'-Azopropane photolysis. Gas-chromatography. Mass-spectrometry.							
82 COW/WAD	EX	333-373	(1.38±0.26)(12)	0	2562±180		2
k_a . trans-2,2'-Azopropane Photooxidation, with or without O_2 . $P(\text{O}_2) = (0-500)$ torr. $P(\text{trans-2,2'-Azoisopropane}) = 5$ torr. $P(\text{N}_2) = (300-500)$ torr.							
79 KIR/PAR	EX	302	(2.15±0.10)(8)				2
k_b . trans-2,2'-Azopropane photolysis. Gas-chromatography. Mass-spectrometry.							
82 COW/WAD	EX	333-373	(2.44±0.31)(10)	0	1443±120		2
k_b . trans-2,2'-Azopropane Photooxidation, with or without O_2 . $P(\text{O}_2) = (0-500)$ torr. $P(\text{trans-2,2'-Azoisopropane}) = 5$ torr. $P(\text{N}_2) = (300-500)$ torr.							
78 KIR/PAR	EX	300-373	(1.43±0.10)(12)	0	2243±60		2
$k_a + k_b$. Azoisopropane/ O_2/N_2 photolysis.							
82 ADA/BAS1	EX	298	(7.8±2.2)(8)				2
$k_a + k_b$. Azoisopropane flash-photolysis at 260 nm. in Ar. $P(\text{Azoisopropane}) = (4.5-10)$ torr. $P(\text{N}_2) = (0-720)$ torr. $P(\text{Ar}) = (0-540)$ torr. $P(\text{Pentane}) = (0-86)$ torr. $P(\text{O}_2) = (2.2-670)$ torr.							
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$							
→ $(\text{CH}_3)_2\text{CHO} +$ 							
Ethyldioxy, 1-methyl- + 2-Butene, 2,3-dimethyl-							
82 SWA/WAD	EX	303-363	9.12(10)	0	4916±214		3.16
Reaction of Isopropylperoxyl with 2,3-Dimethyl-2-butene in a Pyrex vessel. The radicals generated by trans-2,2'-Azopropane/ O_2/N_2 photooxidation. $P(2,3\text{-Dimethyl-2-butene}) = 20$ torr. $P(\text{trans-2,2'-Azoisopropane}) = 5$ torr. $P(\text{O}_2) = (50-450)$ torr. $P(\text{N}_2) = (25-450)$ torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CHO}_2 + (\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 \rightarrow \text{products}$						
Ethylldioxy, 1-methyl- + Propylldioxy, 1,1,2-trimethyl-						
75 ALC/MIL	ES	373	6.2(11)			2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OH} \rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{H}_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}_2\text{O}$ (b)						
$\rightarrow \text{CH}_3 + \text{CH}_2\text{CH}_2\text{OH}$ (c)						
1-Propanol						
71 GON/LEW	EX	753-833	6.80(5)	0	13265	1
$k_a + k_b$.						
76 TSA1	ES	1080-1165	1.58(16)	0	41100	1
k_c .						
$(\text{CH}_3)_2\text{CHOH} \rightarrow (\text{CH}_3)_2\text{CO} + \text{H}_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{H}_2\text{O}$ (b)						
$\rightarrow \text{CH}_3 + \text{CH}_3\text{CHOH}$ (c)						
2-Propanol						
71 GON/LEW	EX	753-833	1.05(5)	0	12582	1
$k_a + k_b$.						
75 TRE	EX	721-801	1.0(14)	0	29039±1007	1 3.98
k_a .						
75 TRE	EX	721-801	1.26(13)	0	29290±1812	1 10.0
k_b .						
76 TSA1	ES	1080-1165	3.16(16)	0	41100	1
k_c .						
\square^{S}	$\rightarrow \text{HCHS} + \text{CH}_2=\text{CH}_2$					
Thietane (Trimethylene sulfide)						
$\rightarrow \text{Methanethial} + \text{Ethene}$						
73 JEF/DAS	EX	980-1040	1.0(13)	0	24258	1
M = Ar.						
Thiethane thermolysis in a single-pulse shock-tube.						
$P_0 = (120-200)$ torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃C(S)OCH₃ → CH₃(O)SCH₃							
Ethanethioic acid O-methyl ester							
72 OEL/TIN Thermal isomerization. T-range not given.	ES		~2.00(13)	0	23402	1	
75 BIG/GAB ¹⁾	EX	629	8.97(-4)			2	
75 BIG/GAB ¹⁾	EX	678-704	7.94(12)	0	23050	1	
¹⁾ Thermal isomerization. Flow reactor pyrolysis.							
 							
Thietane, 1,1-dioxide- (Trimethylenesulfone) → Cyclopropane + Sulfur dioxide							
75 COR/TSA Pyrolysis in a flow-tube reactor.	EX	638-678	1.26(16)	0	28100±500	1	2.0
 CH₂=CHCN + NH₂CH₂CH₂CN → NH(CH₂CH₂CN)₂							
2-Propenenitrile (Acrylonitrile) + Propanenitrile, 3-amino- (β-Aminopropionitrile) → Propanenitrile, 3,3'-iminobis- (β,β'-Iminodipropionitrile)							
82 SAI/MIC Reaction of 2-Propenenitrile with β-Amino- propionitrile in an Autoclave.	EX	303-408	7.43(10)	0	6241	2	
 CH₃CH₂CN → CH₃ + CH₂CN (a) → CH ₂ =CH ₂ + HCN (b) → CH ₂ =CHCN + H ₂ (c)							
Propanenitrile							
78 KIN/GOD ¹⁾ k _a . In presence of excess C ₆ H ₅ NH ₂ .	EX	896-1020	1.77(15)	0	40764	1	
73 DAS/EMO k _b .	EX	803-943	1.29(13)	0	34967±201	1	1.02
78 KIN/GOD ¹⁾ k _b . In absence of additives.	EX	896-1020	2.00(14)	0	34125±806	1	2.51


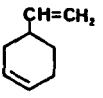
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 KIN/GOD ¹⁾ k _c . In absence of additives.	EX	896-1020	1.26(12)	0	29746±710	1 2.0
¹⁾ Pyrolysis in a flow-reactor. Gas-chromatography. [CH ₃ CH ₂ CN] ~ 6.0x10 ¹⁶ molec.cm ⁻³ . P ~ 760 torr.						
$\triangle_{\text{NH}_2} \rightarrow (\text{CH}_3\text{CH}=\text{CHNH}_2 = \text{CH}_3\text{CH}_2\text{CH}=\text{NH})$						
Cyclopropanamine						
→ (1-Propen-1-amine = 1-Propanimine)						
73 PAR/ROB Thermal isomerization in a silica reaction vessel with Pyrex vacuum-system. Gas-chromatography. The intermediate product reacts with another molecule of reactant to form one molecule of:	EX	629-698	1.15(15)	0	29109±313	1 2.57
$\triangle_{\text{N}=\text{CHCH}_2\text{CH}_2}$						
(Cyclopropanamine, N-propylidene-).						
P ₀ = (15-60) torr.						
(CH ₃) ₂ CHONO → (CH ₃) ₂ CO + HNO (a) → CH ₃ CH=CH ₂ + HONO (b) → (CH ₃) ₂ CHO + NO (c)						
Nitrous acid 1-methylethyl ester (Isopropyl nitrite)						
75 BAT/MCC k _a .	ES	393-473	1.26(9)	0	13437	1
77 BAT/MIL1 k _a .	ES	403-433	2.51(9)	0	13588	1
78 BAT/ISL2 ¹⁾ k _a .	EX	433-473	2.00(14)	0	19577±503	1 3.16
78 BAT/ISL2 ¹⁾ k _b .	EX	433-473	5.01(12)	0	19074	1
¹⁾ Pyrolysis in a static system. Gas-liquid chromatography.						
77 BAT/MIL1 k _c . Same data given in 74 BAT/MIL and 75 BAT/MCC.	ES	403-433	1.58(16)	0	20634±403	1 2.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

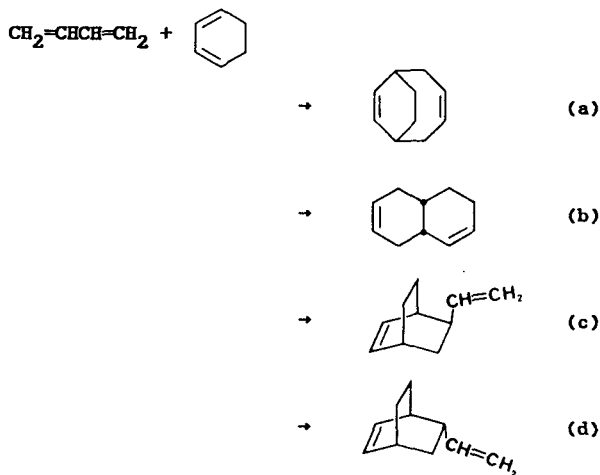
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
CH₃NHC(O)OCH₃ → CH₃NCO + CH₃OH						
Carbamic acid, methyl-, methyl ester						
72 DAL/ZIO1 Thermolysis.	EX	643-695	2.45(12)	0	24187	1
CH₃CH₂CH₂ONO₂ → CH₃CH₂CH₂O + NO₂						
Nitric acid propyl ester (n-Propyl nitrate)						
75 MEN/GOL RRKM fit of experimental data.	CO	300	3.15(16)	0	20131	1
77 BAR/BEN2 VLP-pyrolysis. RRKM best-fit estimate.	EX	580-800	3.16(16)	0	20131	1
CH=CC=C → C=CC=C + H						
1,3-Butadiynyl						
80 FRA/JUS Thermolysis of Ethyne and 1,3-Butadiyne in Ar, behind shock-waves. Data-fit on the basis of a proposed mechanism. Total Conc. = (0.4-1.6)x10 ¹⁹ molec.cm ⁻³ .	ES	2100-2300	(1.35±0.85)(14)	0	58700	1
CH=CC=C + CH=CC=CH → CH=CC=CC=CH + H						
1,3-Butadiynyl + 1,3-Butadiyne						
80 FRA/JUS Thermolysis of Ethyne and 1,3-Butadiyne in Ar, behind shock-waves. Data-fit on the basis of a proposed mechanism. Total Conc. = (0.4-1.6)x10 ¹⁹ molec.cm ⁻³ .	ES	1850-2300	(3.5±2.0)(13)	0	0	2
CH=CC=CH → CH=CC=C + H						
1,3-Butadiyne						
80 FRA/JUS Thermolysis of Ethyne and 1,3-Butadiyne in Ar, behind shock-waves. Total Conc. = (0.4-1.6)x10 ¹⁹ molec.cm ⁻³ .	ES	1850-2300	(2.2±0.6)(14)	0	58700±700	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CH₂C≡CH → CH₃ + CH₂C≡CH							
1-Butyne							
78 KIN VLP-pyrolysis.	EX	1052-1152	3.16(15)	0	37343±1007	1	2.0
82 TRE/WRI Pyrolysis of 1-Butyne in a cylindrical silica reaction vessel with static system. Gas-chromatography. P = (50-1200) torr.	EX	652-731	1.58(17)	0	37645±1057	1	5.01
CH₃CH₂C≡CH + CH₃CH₂C≡CH → CH₃CH₂C=CH₂ + CH₃CHC≡CH							
1-Butyne							
82 TRE/WRI Rate determining step. CH ₃ CH ₂ C=CH ₂ decomposes further to give CH ₃ and CH ₂ =C=CH ₂ . Pyrolysis of 1-Butyne in a cylindrical silica reaction vessel with static system. Gas-chromatography. P = (50-1200) torr.	EX	652-731	2.00(14)	0	24056±302	2	1.58
CH₂=CHCH=CH₂ + CH₂=CHCH=CH₂							
	→		(a)				
	→		(b)				
1,3-Butadiene							
77 HUY/LUY ¹⁾ k _a .	EX	464-557	4.47(10)	0	14313±50	2	1.10
77 HUY/LUY ¹⁾ k _b .	EX	464-557	8.91(9)	0	12345±60	2	1.12
¹⁾ Thermal reaction of 1,3-Butadiene in a static system. Gas-chromatography. P = (49-450) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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1,3-Butadiene + 1,3-Cyclohexadiene

- \rightarrow Bicyclo[4.2.2]deca-3,7-diene (a)
- \rightarrow Naphthalene, 1,2,4a,5,8,8a-hexahydro-, cis- (b)
- \rightarrow Bicyclo[2.2.2]oct-2-ene, 5-ethenyl- ($1\alpha, 4\alpha, 5\alpha$)- (exo form) (c)
- \rightarrow Bicyclo[2.2.2]oct-2-ene, 5-ethenyl- ($1\alpha, 4\alpha, 5\beta$)- (endo form) (d)

82 HUY/HUB2 ¹⁾ k_a .	EX	437-526	4.07(9)	0	12849±25	2	1.05
82 HUY/HUB2 ¹⁾ k_b .	EX	437-526	1.05(10)	0	12768±35	2	1.07
82 HUY/HUB2 ¹⁾ k_c .	EX	437-526	1.055(10)	0	13468±25	2	1.05
82 HUY/HUB2 ¹⁾ k_d .	EX	437-526	3.80(9)	0	12501±25	2	1.05

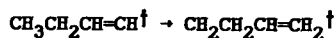
¹⁾ Thermal Diels-Alder addition

in a static system.

Gas-chromatography.

P(1,3-Cyclohexadiene) = (50-93) torr.

P(1,3-Butadiene) = (61-397) torr.



1-Butenyl \rightarrow 3-Butenyl

76 IBU/TSU ¹⁾	EX	348	1.00(9)				1
76 IBU/TSU ¹⁾	EX	396	1.05(9)				1

¹⁾ Photolysis of 3-Pentanone.

$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}^\dagger$ formed by $\text{CH}_3\text{CH}_2 + \text{CH}=\text{CH}$.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}=\text{CHCH}_2 + \text{H}_2\text{S} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{SH}$ 2-Butenyl + Hydrogen sulfide	ES	750-816	1.0(14)	0	4680	2
80 RIC/BOI Static system. cis/trans-Butenyl equilibrium.						
$\text{CH}_3\text{CH}=\text{CHCH}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_3$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CHCH}_2$ 2-Butenyl + 2-Butene, (Z)-	RL	750-816	4.0(-1)	0	3271±503	2/2
80 RIC/BOI ¹⁾ $k_{\text{ref}}: \text{CH}_3\text{CH}=\text{CHCH}_2 + \text{H}_2\text{S} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{SH}$	ES	750-816	≈3.98(13)	0	7952	2
80 RIC/BOI ¹⁾ 1) Static system. cis/trans-Butenyl equilibrium.						
$\text{trans-CH}_3\text{CH}=\text{CHCH}_2 \rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_2$ 2-Butenyl, (E)-	RL	363	(1.64±0.28)(-6)			1/2
72 GOR/WAL $k_{\text{ref}}: \text{trans-CH}_3\text{CH}=\text{CHCH}_2 + \text{HI}$ $\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{I}$ (a) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{I}$ (b)	ES	363	5.01(4)			1
72 GOR/WAL						
$\text{CH}_2=\text{CHCH}_2\text{CH}_2^\ddagger \rightarrow [\text{CH}_3\text{CHCH}=\text{CH}_2^\ddagger = \text{CH}_3\text{CH}=\text{CHCH}_2^\ddagger]$ 3-Butenyl → [2-Propenyl, 1-methyl- = 2-Butenyl]	EX	348	3.47(7)			1
76 IBU/TSU ¹⁾	EX	396	6.20(7)			1
76 IBU/TSU ¹⁾ 1) Photolysis of 3-Pentanone. $\text{CH}_2=\text{CHCH}_2\text{CH}_2^\ddagger$ formed by isomerization of $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}^\ddagger$, which (in its turn) was formed by $\text{CH}_3\text{CH}_2 + \text{CH}=\text{CH}$.						
$\text{CH}_2=\text{CHCH}_2\text{CH}_2 + \square^\circ$						
$\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \square$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \square$ (b)						
$\rightarrow \begin{array}{c} \text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \\ \square \end{array}$ (c)						
3-Butenyl + Cyclobutyl	RL	298	(1.3±0.5)(-1)			2/2
75 STE/RAB ¹⁾ k_a/k_c .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 STE/RAB ¹⁾ k _b /k _c .	RL	298	(3.0±0.9)(-1)			2/2
75 STE/RAB ¹⁾ (k _a + k _b)/k _c .	RL	298	(4.3±0.7)(-1)			2/2
¹⁾ Disproportionation-combination ratios.						
CH ₃ C=CHCH ₃ [†] → CH ₃ C=CH + CH ₃ (a) → CH ₃ C=CCH ₃ + H (b)						
1-Propenyl, 1-methyl- → 1-Propyne + Methyl (a) → 2-Butyne + Hydrogen atom (b)						
77 DIA/DOE ¹⁾ k _a /k _{ref} .	RL	298	(3.70±1.02)			1/1
77 DIA/DOE ¹⁾ k _b /k _{ref} .	RL	298	5.04			1/1
¹⁾ Study of the UV-photolysis of 1,2-Butadiene. CH ₃ C=CHCH ₃ [†] formed by H + CH ₃ =C=CH ₂ . k _{ref} : CH ₂ =CCH ₂ CH ₃ [†] → CH ₂ =C=CH ₂ + CH ₃						
CH ₂ =CHCHCH ₃ [†] → CH ₂ =CHCH=CH ₂ + H						
2-Propenyl, 1-methyl- (1-Methylallyl) → 1,3-Butadiene + Hydrogen atom						
77 DIA/DOE k/k _{ref} . Study of the UV-photolysis of 1,2-Butadiene. CH ₂ =CHCHCH ₃ [†] formed by H + CH ₃ =C=CH ₂ . k _{ref} : CH ₂ =CCH ₂ CH ₃ [†] → CH ₂ =C=CH ₂ + CH ₃	RL	298	(1.86±0.01)			1/1
trans-CH ₃ CHCH=CH ₂ → cis-CH ₃ CHCH=CH ₂						
2-Propenyl, 1-methyl-, (E)- (trans-1-Methylallyl)						
72 GOR/WAL	ES	363	5.0(4)			1
CH ₂ =CHCHCH ₃ + CH ₂ =CHCHCH ₃ → CH ₂ =CHCH(CH ₃)CH(CH ₃)CH=CH ₂						
2-Propenyl, 1-methyl- (1-Methylallyl)						
78 BAY 3-Methyl-1-butene, cis-2-Pentene, 1-Butene and trans-2-Butene Flash-photolysis. Kinetic Spectroscopy. Gas-chromatography.	EX	295	(3.5±0.4)(13)			2
CH ₂ C(CH ₃)=CH ₂ → CH ₂ =C=CH ₂ + CH ₃						
2-Propenyl, 2-methyl- (2-Methylallyl)						
73 TSA2 1050 K given by the author as central-T.	EX	996-1180	2.14(13)	0	25200±400	1 1.58

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2 + \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2$ $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$						
2-Propenyl, 2-methyl- (2-Methylallyl)						
73 BAY/BRO	EX	295	(2.6±0.3)(13)			2
73 TSA2	ES	996-1180	5.01(12)			2 3.98
1020 K given by the author as central-T.						
76 BAY	EX	295	(2.6±0.3)(13)			2
2-methyl-1-butene and 2-methyl-1-propene						
Kinetic Spectroscopy.						
Flash-Photolysis.						
$\square^\bullet + \square^\bullet \rightarrow \square + \square \quad (\text{a})$ $\rightarrow \text{Cyclobutane} \quad (\text{b})$						
Cyclobutyl						
75 STE/RAB	RL	298	(1.33±0.10)			2/2
k_a/k_b .						
Disproportionation-combination ratio.						
$\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_2\text{CH}=\text{CH}_2 \quad (\text{a})$ $\rightarrow \text{any other products (b)}$						
1-Butene						
81 AYR/BAC	RL	750	6.31(-1)	0	2214	1/2
k_a/k_{ref} .						
Pyrolysis in a static system.						
$k_{\text{ref}}: \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2 \rightarrow \text{CH}_2=\text{CH} + \text{CH}_3\text{CH}_2$						
73 SHI/KIN2	EX	829-1040	1.26(13)	0	29963	1
k_{overall} .						
$\text{cis-CH}_3\text{CH}=\text{CHCH}_3 (+ \text{M}) \rightarrow \text{CH}_3\text{CH}=\text{CHCH}_2 + \text{H} (+ \text{M}) \quad (\text{a})$ $\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{H}_2 (+ \text{M}) \quad (\text{b})$ $\rightarrow \text{CH}_2=\text{CHCH}_2 + \text{CH}_3 (+ \text{M}) \quad (\text{c})$ $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 (+ \text{M}) \quad (\text{d})$						
2-Butene, (Z)-						
80 RIC/BOI	ES	750-816	≈3.16(15)	0	43030	1
k_a .						
Conventional static system.						
Mass-spectrometry.						
73 ALF/GOL	DE	1100-1300	1.0(13)	0	32713±1007	1 3.98
k_b .						
RRKM fit of experimental data.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
76 MAS/RIC k _b . Static system. Same data given in 76 RIC/MAR. P ₀ ~ 50 torr.	EX	480-550	1.0(13)	0	32964±1007	1	3.16
74 JEF/BAU k _c . Average k.	RN	1150-1325	1.0(16)	0	40262	1	
74 JEF k _d . Shock-tube cis-trans isomerization.	EX	990-1300	2.51(14)	0	33317	1	1.58
76 MAS/RIC k _d . Static system. Limiting high-pressure k. P ₀ = ~ 50 torr. Same data given in 76 RIC/MAR.	EX	753-823	3.98(13)	0	31203±503	1	2.0
73 COX k _d . M = SO ₂ (³ B ₁). 59% trans isomer formed.	RN	296	(1.62±0.08)(14)			2	
74 SPR/AKI k _d . M = NO ₂ .	EX	298-366	7.26(10)	0	5944±42	2	1.14
cis-CH ₃ CH=CHCH ₃ + H ₂ S → CH ₃ CH ₂ CHCH ₃ + SH							
2-Butene, (Z)- + Hydrogen sulfide							
80 RIC/BOI ¹⁾ k _{ref} : cis-CH ₃ CH=CHCH ₃ → CH ₃ CH=CHCH ₂ + H	ES	750-816	1.29(-2)	0	16004	2/1	
80 RIC/BOI ¹⁾	ES	750-816	3.98(13)	0	27026	2	
¹⁾ Static system. Mass-spectrometry.							
trans-CH ₃ CH=CHCH ₃ (+ M) → CH ₃ + CH ₂ =CHCH ₂ (+ M) (a)							
→ cis-CH ₃ CH=CHCH ₃ (+ M) (b)							
2-Butene, (E)-							
74 JEF/BAU k _a . Average k.	EX	1150-1325	1.0(16)	0	40262	1	
73 COX k _b . M = SO ₂ (³ B ₁). 41% cis isomer formed.	EX	296	(1.42±0.09)(14)			2	
74 SPR/AKI k _b . M = NO ₂ .	EX	297-370	4.49(10)	0	6135±59	2	1.21
(CH ₃) ₂ C=CH ₂ → CH ₃ + CH ₂ CH=CH ₂ (a)							
→ any other products (b)							
1-Propene, 2-methyl-							
76 BRA/WES2 k _a . Optimization by computer simulation on the basis of a proposed mechanism.	DE	1055-1325	1.82(18)	0	45107	1	1.23

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
74 BAK/NOV k _{overall} .	EX	973-1123	1.14(16)	0	38752±1258	1
71 KOR/KAL k _{overall} . Pyrolysis in a quartz reactor. Gas-chromatography. P(Total) = 100 torr.	EX	1070-1200	1.89(16)	0	3976	1 1.2
$\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2$ (a)						
→ \square (b)						
1,4-Butanediyl → Ethene + Ethene (a)						
→ Cyclobutane (b)						
72 BEA/GOL1 ¹⁾ k _a .	ES	969-1280	1.17(13)	0	4152	1
72 BEA/GOL1 ¹⁾ k _b .	ES	969-1280	2.0(12)	0	3320	1
¹⁾ Cyclobutane/Ar VLP-Pyrolysis. Mass-spectrometry.						
$\square \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ (a)						
→ $\text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{CH}_2$ (overall) (b)						
Cyclobutane → 1,4-Butanediyl (a)						
→ Ethene + Ethene (b)						
72 BEA/GOL1 ¹⁾ k _a .	ES	969-1280	3.63(15)	0	31877	1
72 BEA/GOL1 ¹⁾ k _b . Least squares treatment. RRKM data-fit.	EX	969-1280	2.63(15)	0	31203	1
72 BEA/GOL1 ¹⁾ k _b . Best value based on the present experiments and all previously reported data.	SE	969-1280	3.16(16)	0	32969	1
¹⁾ Cyclobutane/Ar VLP-Pyrolysis. Mass-spectrometry. Extrapolated limiting high-pressure k's.						
74 BAR/COC ²⁾	EX	891	6.03			1
74 BAR/COC ²⁾	EX	955	6.13(1)			1
74 BAR/COC ²⁾	EX	1000	1.26(2)			1
74 BAR/COC ²⁾	EX	1231	4.38(3)			1
74 BAR/COC ²⁾	EX	1400	1.13(4)			1
²⁾ k _b . M = Ar. Cyclobutane thermolysis behind reflected shock-waves in a single-pulse shock-tube.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
[Cyclobutane] = (0.2-1.0)%. Limiting high-pressure k.						
Other rate constants at various temperatures within the 891-1400 K range are tabulated.						
The Arrhenius plot shows a pronounced curvature in the vicinity of 1080 K.						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_2=\text{CH}_2$						
Butyl						
80 GAW/GIE ¹⁾ At 313 nm. Experimental data-fit by using the Stern-Volmer equation.	EX	298	3.2(9)			1
80 GAW/GIE ¹⁾ At 313 nm. RRKM calculation.	CO	298	3.1(9)			1
80 GAW/GIE ¹⁾ At 334 nm. Experimental data-fit by using the Stern-Volmer equation.	EX	298	1.2(9)			1
80 GAW/GIE ¹⁾ At 334 nm. RRKM calculation.	CO	298	1.05(9)			1
¹⁾ HI irradiation with UV-light. Reaction of hot H atoms with 1-Butene in a Pyrex vacuum-system. P = (0.4-400) torr.						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 + \text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{HO}_2$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O}_2$ (b)						
Butyl + Oxygen molecule						
71 BAK/BAL k_a/k_{ref} $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$	ES	753	1.57(6)			2/1
71 BAK/BAL k_a	ES	753	2.8(11)			2
80 LEN/MCD k_b . M = He. 1-Iodobutane flash-photolysis. Photoionization Mass-spectrometer. Limiting high-pressure k. P-independent for (1-4) Torr range.	EX	298	(4.52±0.84)(12)			2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2$						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (b)						
Butyl						
71 FAL/SUN k_a/k_b	RL	298	1.4(-1)			2/2


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
<hr/>						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)$						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ (b)						
Butyl + Propyl, 1-methyl-						
71 FAL/SUN	RL	298	4.5(-1)			2/2
k_a/k_b .						
<hr/>						
$\text{CH}_3\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$						
Propyl, 1-methyl-						
80 GAW/GIE ¹⁾	EX	298	2.5(9)			1
At 313 nm. Stern-Volmer experimental data-fit.						
80 GAW/GIE ¹⁾	CO	298	2.58(9)			1
At 313 nm. RRKM calculation.						
80 GAW/GIE ¹⁾	EX	298	1.05(9)			1
At 334 nm. Experimental data-fit by using the Stern-Volmer equation.						
80 GAW/GIE ¹⁾	CO	298	9.14(8)			1
At 334 nm. RRKM calculation.						
¹⁾ HI irradiation with UV-light. Reaction of hot H atoms with 1-Butene in a Pyrex vacuum system. P = (0.4-400) torr.						
<hr/>						
$\text{CH}_3\text{CH}_2\text{CHCH}_3 + \text{O}_2 \rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{HO}_2$ (a)						
$\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{HO}_2$ (b)						
$\rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{OH}$ (c)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{OO}\cdot)\text{CH}_3$ (d)						
Propyl, 1-methyl- + Oxygen molecule						
71 BAK/BAL ¹⁾	RL	753	5.40(5)			2/1
k_a/k_{ref} .						
71 BAK/BAL ¹⁾	RL	753	9.63(5)			2/1
k_b/k_{ref} .						
¹⁾ k_{ref} : $\text{CH}_3\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$						
71 BAK/BAL	ES	753	1.2(11)			2
k_a .						
71 BAK/BAL	ES	753	2.1(11)			2
k_b .						
71 BAK/BAL	ES	753	2.3(11)			2
k_c .						
80 LEN/MCD	EX	298	(1.00±0.13)(13)			2
k_d . M = He. 2-Iodobutane flash-photolysis. Photoionization Mass-spectrometer. Limiting high-pressure k. P-independent for (1-4) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CH}_2\text{CHCH}_3 + \text{CH}_3\text{CH}_2\text{CHCH}_3$							
→ $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (a)	(a)						
→ <i>cis</i> - $\text{CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (b)	(b)						
→ <i>trans</i> - $\text{CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ (c)	(c)						
→ $\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{H}_2\text{CH}_3$ (d)	(d)						
Propyl, 1-methyl-							
71 FAL/SUN k_a/k_d .	RL	298	(4.1±0.2)(-1)				2/2
71 FAL/SUN ($k_b + k_c$)/ k_d .	RL	298	(3.6±0.3)(-1)				2/2
71 FAL/SUN ($k_a + k_b + k_c$)/ k_d .	RL	298	(7.7±0.5)(-1)				2/2
$(\text{CH}_3)_2\text{CHCH}_2 + \text{O}_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HO}_2$ (a)							
→ $(\text{CH}_3)_2\text{CHCHO} + \text{OH}$ (b)							
Propyl, 2-methyl- + Oxygen molecule							
71 BAK/BAL ¹⁾	ES	753	8.92(5)				2/1
78 BAK/BAL ¹⁾ ³⁾	RL	753	(7.75±1.00)(5)				2/1
¹⁾ k_a/k_{ref} .							
k_{ref} : $(\text{CH}_3)_2\text{CHCH}_2 \rightarrow \text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$							
71 BAK/BAL ²⁾	ES	753	2.3(10)				2
78 BAK/BAL ²⁾ ³⁾	RN	753	(6.8±3.4)(10)				2
78 BAK/BAL ²⁾ ³⁾	ES	313-753	4.7(12)	0	3200		2
²⁾ k_a .							
³⁾ Oxidation in aged boric-acid-coted vessels. P(Total) = (490-505) torr.							
71 BAK/BAL k_b .	ES	753	2.3(9)				2
$(\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}$ (a)							
→ $\text{CH}_3 + \text{CH}_3\text{CH}=\text{CH}_2$ (b)							
→ $\text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}_2$ (c)							
Ethyl, 1,1-dimethyl (t-Butyl)							
81 CAN/MAR2 k_a . Azomethane-sensitized pyrolysis of Isobutane in a static system. P(Total) = (53-270) torr.	EX	584-604	4.68(14)	0	19829		1
76 BRA/WES1 ¹⁾	RL	1030-1300	7.2(3)	0	11078	1/1	1.32
76 BRA/WES2 ¹⁾	RL	1055-1325	1.27(-2)	0	-5846	1	1.41
76 BRA/WES2 ¹⁾	RL	1200	1.8				1/1
¹⁾ k_b/k_c .							
Fit of experimental data to a proposed mechanism by computer optimization.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{C} + \text{O}_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HO}_2$ (a) $\rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3 + \text{O}$ (b) $\rightarrow (\text{CH}_3)_3\text{COO}$ (c)						
Ethyl, 1,1-dimethyl- (t-Butyl) + Oxygen molecule						
78 ATR/BAL k_a . Oxidation in KCl-coated vessels. P = (60-500) torr. k_{ref} : $(\text{CH}_3)_3\text{C} + \text{O}_2 \rightarrow$  + OH	EX	470-542	1.38(1)	0	-1564	2/2
79 EVA/WAL ¹⁾ k_a/k_{ref} . k_{ref} : $(\text{CH}_3)_3 + \text{H}_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}$	RL	713-813	(3.5±1.0)(-1)	0	-7446±241	2/2
79 EVA/WAL ¹⁾ k_a . ¹⁾ Oxidation in KCl-coated reaction vessels.	RN	713-813	8.0(11)	0	1095±1203	2
80 WAS/BAY $(k_a + k_b)/k_{\text{ref}}$. Fast-flow reactor. Photoionization Mass-spectrometer. k measurements by Stern-Volmer plots. Channels (a) and (b) assumed to be not elementary, but to pass first through channel (c) to form the t-Butylperoxy radical which in its turn reacts with an O atom to form either Isobutene + O ₂ , or Acetone + Methyl + O ₂ . P(Isobutane) = (2.7-4.2) mtorr. P(Total) = (1.8-5.7) torr. P(O) ₀ = (4.3-8.5) mtorr. k_{ref} : $(\text{CH}_3)_3\text{C} + \text{O} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{OH}$ (c) $\rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3$ (d)	RL	297	(2.68±0.36)(-2)			2/2
80 LEN/MCD k_c . M = He. 2-Iodo-2-methylpropane flash-photolysis. Photoionization Mass-spectrometry. P-independent for (1-4) torr. Limiting high-pressure k.	EX	298	(1.41±0.23)(13)			2
$(\text{CH}_3)_3\text{C} + \text{O}_3 \rightarrow$ products Ethyl, 1,1-dimethyl- (t-Butyl) + Ozone						
82 PAL Photoionization mass-spectrometry. $(\text{CH}_3)_3\text{C}$ generated by photodissociation of 2,4,4-Trimethylpent-1-ene. P = 2 torr.	EX	298	(3.28±0.29)(13)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{C} + \text{H}_2 \rightarrow (\text{CH}_3)_3\text{CH} + \text{H}$						
Ethyl, 1,1-dimethyl- (t-Butyl) + Hydrogen molecule						
79 EVA/WAL Reaction in KCl-coated vessels.	DE	713-813	2.3(12)	0	8540±720	2
$(\text{CH}_3)_3\text{C} + \text{NO} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HNO}$ (a)						
$\rightarrow (\text{CH}_3)_3\text{CNO}$ (b)						
Ethyl, 1,1-dimethyl- (t-Butyl) + Nitrogen oxide (NO)						
74 CHO/MEN k_a . Upper-limit k.	EX	600	≤3.16(10)			1
74 CHO/MEN k_b .	EX	600	(3.5±1.7)(12)			1
$(\text{CH}_3)_3\text{C} + (\text{CH}_3)_3\text{C} \rightarrow (\text{CH}_3)_2\text{CH}=\text{CH}_2 + (\text{CH}_3)_3\text{CH}$ (a)						
$\rightarrow (\text{CH}_3)_3\text{CC}(\text{CH}_3)_3$ (b)						
Ethyl, 1,1-dimethyl- (t-Butyl)						
71 FAL/SUN ¹⁾	RL	298	3.1			2/2
74 CHO/BEA ¹⁾	RL	620-690	3.0	0	0	2/2
76 PAR/QUI ¹⁾	RL	298	(2.8±0.2)			2/2
77 MCK/TUR ¹⁾ Thermolysis in a vacuum system. Average ratio.	RL	483-515	(2.6±0.04)	0	0	2/2
77 MAR/MAC ¹⁾ Thermolysis in a vacuum system. Average ratio.	RL	483-533	(2.9±0.2)	0	0	2/2
81 BET/LAN ^{1) 4)}	RL	298	(2.9±0.2)			2/2 2.0
¹⁾ $k_a/k_b = k_{\text{dispr.}}/k_{\text{comb.}}$						
74 CHO/BEA ²⁾	EX	620-690	1.5(12)	0	0	2
81 BET/LAN ^{2) 4)} ²⁾ k_a .	EX	298	1.35(13)			2 2.0
72 MCM/GOL ³⁾	EX	462	3.98(8)			2
73 HIA/BEN ³⁾	ES	373	2.51(8)			2
73 KON/MAR ³⁾	ES	773	3.98(9)			2
74 CHO/BEA ³⁾	EX	620-690	5.0(11)	0	0	2 2.0
75 PAR/QUI ³⁾	RN	298	(1.2±0.18)(12)			2
81 BET/LAN ^{3) 4)} ³⁾ k_b .	EX	298	4.68(12)			2 2.0
81 BET/LAN ⁴⁾ $k_a + k_b$.	EX	298	1.82(13)			2 2.0
⁴⁾ Time-resolved Infrared Spectral Photography. Gas-chromatography. Mass-spectrometry. P[(CH ₃) ₃ NO] = (15-30) torr. P(NO) = (3-17.5) torr.						


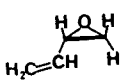

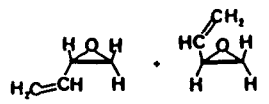
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 DEM/LDE $k_a + k_b$. Flash-photolysis. Laser-resonance-absorption. (CH ₃) ₃ C generated by flashing NH ₃ in presence of Isobutene. Data-simulation. Best-fit.	DE	298	6.5(12)			2
CH ₃ CH ₂ CH ₂ CH ₃ → CH ₃ CH ₂ + CH ₃ CH ₂ (a) → CH ₃ CH ₂ CH ₂ + CH ₃ (b)						
Butane						
74 GOL/ALF ¹⁾ RRKM calculation. Best fit of experimental data.	DE	1100-1250	2.51(16)	0	40715	1
74 HUG/MAR ¹⁾	ES	895-981	2.0(15)	0	38852±2044	1 7.94
78 TSA4 ¹⁾ Single-pulse shock-tube.	EX	990-1100	2.51(16)	0	41300	1
78 TSA4 ¹⁾ Extrapolation over the given T-range. Single-pulse shock-tube.	EX	300-1100	1.58(17)	0	43800	1
79 PRA/ROG3 ¹⁾ M = Ar. Butane pyrolysis in a wall-less reactor. P(Ar) = 600 torr.	EX	1025	(3.8±0.6)(-2)			1
¹⁾ k_a .						
74 HUG/MAR ²⁾	EX	895-981	2.57(15)	0	38853±1804	1 6.76
72 HAS/JOH ²⁾ P = 0.35 torr. Butane vibrationally excited.	EX	298	(7.3±0.6)(6)			1
72 HAS/JOH P = 1.06 torr. Butane vibrationally excited.	EX	298	(2.3±0.2)(7)			1
80 SHE/IVA ²⁾ Pyrolysis in a quartz reactor. Initial steps of a proposed mechanism. P = 100 torr.	EX	973-1123	1.74(14)	0	31480±1384	1 3.80
²⁾ $k_a + k_b$.						
81 KOI/MOR2 k_b . M = Ar. Pyrolysis of Butane behind incident shock-waves. P = 20 torr.	EX	1290-1610	8.9(13)	0	36185	1
72 ILL ³⁾	EX	913-1063	5.82(12)	0	28430	1
72 ILL/SZA ³⁾	EX	940-1075	2.45(13)	0	30201	1 1.1
74 BAK/NOV ³⁾	EX	973-1123	1.5(12)	0	26774±805	1
³⁾ k_{overall} .						
(CH ₃) ₃ CH → (CH ₃) ₂ CH + CH ₃ (a) → any other products (b)						
Propane, 2-methyl- (Isobutane)						
73 KON/MAR k_a . Estimated k.	RE	770-855	6.31(16)	0	41117	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
74 GOL/ALF k _a . RRKM calculation. Best fit of data.	DE	1100-1280	2.51(16)	0	41671	1	
80 PRA/ROG ¹⁾	EX	1000	(1.8±0.5)(3)			1	
80 PRA/ROG ¹⁾ Determined on the basis of the experimental k at 1000 K and thermodynamic data.	DE	970-1031	8.4(15)	0	42985	1	
¹⁾ k _a . M = Ar. Isobutane pyrolysis in a wall-less reactor. P(Ar) = 600 torr.							
82 KOI/MOR2 k _a . M = Ar. Pyrolysis of Isobutane behind incident shock-waves. UV-Absorption spectroscopy. P(Total) = 380 torr.	EX	1300-1800	6.31(12)	0	30599±2315	1	3.16
80 SHE/IVA k _a . Pyrolysis in a quartz reactor. Initial step of a proposed mechanism. P = 100 torr.	EX	973-1123	1.66(11)	0	24308±1158	1	3.02
72 ILL k _{overall} .	EX	913-1063	1.10(15)	0	33644	1	
78 VER/BEL k _{overall} /k _{ref} . Pyrolysis in a flow-reactor. k _{ref} : CH ₃ CH ₂ CH ₂ CH ₃ → products. Average ratio.	RL	985-1073	(9.25±0.95)(-1)			1/1	
(CH ₃) ₃ CH [†] → (CH ₃) ₂ CH + CH ₃ Propane, 2-methyl- (Isobutane)							
71 LEX/MAR2 Discharge flow. Upper-limit ratio. (CH ₃) ₃ CH [†] formed by H + (CH ₃) ₃ C. The rate ratio given by the authors is: k/k _{ref} = (2±22)×10 ⁻¹⁰ mol.cm ⁻³ . k _{ref} : (CH ₃) ₃ CH [†] + M → (CH ₃) ₃ CH + M. P(Ar) = (4-12) torr.	RL	290	<2.46(-9)			1/2	
CH=CCH ₂ COOH → CH ₂ =C=CH ₂ + CO ₂ 3-Butynoic acid							
76 BIG/WEA1	EX	630	1.49(-2)			1	
76 BIG/WEA1 A and B recalculated from the reported data.	EX	500-648	2.21(11)	0	19106±758	1	
CH=CCH ₂ COOD → CHD=C=CH ₂ + CO ₂ 3-Butynoic acid-d							
76 BIG/WEA1	EX	630	5.08(-3)			1	


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2\text{C}(\text{O})\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_2=\text{C}=\text{O} + \text{CH}_3\text{CO}$ Butyl, 2,3-dioxo-	EX	822-905	2.00(15)	0	26170	1	
75 SCH/PLA							
 $\rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{C}=\text{O}$ (a)							
$\rightarrow \triangle + \text{CO}$ (b)							
Cyclobutanone							
72 MCG/SCH ¹⁾	EX	633-679	3.6(14)	0	26120	1	
k_a .							
72 MCG/SCH ¹⁾	EX	633-679	6.3(13)	0	28334	1	
k_b .							
¹⁾ Pyrolysis in a high-vacuum static system. Gas-chromatography. $P_0 = (1.5-38)$ torr.							
 \rightarrow  (a)							
\rightarrow  (b)							
(Racemic mixture)							
Oxirane, ethenyl-, (S)-							
\rightarrow Furan, 2,3-tetrahydro- (a)							
\rightarrow Oxirane, ethenyl-, (±)- (racemic) (b)							
76 CRA/LUT ¹⁾	EX	543-583	2.00(14)	0	25466±604	1	7.94
k_a .							
Ring expansion.							
76 CRA/LUT ¹⁾	EX	528-548	3.39(13)	0	22245±352	1	2.0
k_b .							
Racemization of the (+)-(S) form.							
$P_0 = 380$ torr.							
76 CRA/LUT ¹⁾	EX	543-583	1.26(14)	0	24056±554	1	6.31
k_{overall} .							
Thermolysis at 114 torr.							
76 CRA/LUT ¹⁾	EX	580	(1.25±0.01)(-4)			1	
k_{overall} .							
¹⁾ Thermolysis in a static system. Mass-spectrometry.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
<p>(a)</p>						
<p>(b)</p> <p>(Racemic mixture)</p>						
<p>(c)</p>						
<p>Oxirane-d, 3-ethenyl-, cis-, (S)-</p> <p>→ Furan-5-d, 2,3-dihydro- (a)</p> <p>→ Oxirane-d, 3-ethenyl-, cis-, (±)- (racemic) (b)</p> <p>→ Oxirane-d, 3-ethenyl-, trans- (c)</p>						
<p>76 CRA/LUT ¹⁾</p> <p>k_a.</p> <p>Ring expansion.</p>	EX	580	1.58(-5)			1
<p>76 CRA/LUT ¹⁾</p> <p>k_b.</p> <p>Racemization of the (+)-(S) form.</p>	EX	580	7.24(-4)			1
<p>76 CRA/LUT ¹⁾</p> <p>k_c.</p> <p>Cis-trans isomerization.</p>	EX	580	1.7(-5)			1
<p>76 CRA/LUT ¹⁾</p> <p>$k_{overall}$.</p> <p>Thermolysis at 114 torr.</p>	EX	580	(1.06±0.01)(-4)			1
<p>¹⁾ Thermolysis in a static system.</p> <p>Mass-spectrometry.</p>						
<p>(a)</p>						
<p>→ any other products (b)</p>						
<p>Oxirane-d, 3-ethenyl-, trans-</p> <p>→ Oxirane-d, 3-ethenyl-, cis- (a)</p> <p>→ any other products (b)</p>						
<p>76 CRA/LUT ¹⁾</p> <p>k_a.</p> <p>Trans-cis isomerization.</p>	EX	580	1.8(-5)			1
<p>76 CRA/LUT ¹⁾</p> <p>$k_{overall}$.</p> <p>Thermolysis at 114 torr.</p>	EX	580	(1.07±0.01)(-4)			1
<p>¹⁾ Thermolysis. Static system. Mass-spectrometry.</p>						

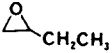

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 \rightarrow products						
Oxirane, 2,2-d ₂ , 3-ethenyl- \rightarrow products						
76 CRA/LUT	EX	580	(9.8±0.1)(-5)			1
Thermolysis. Static system. Mass=spectrometry. P = 114 torr.						
$\text{CH}_2=\text{CHCH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2$						
3-Butenoic acid						
82 BIG/CLA ¹⁾	EX	634	5.0(-3)			1
P(Total) _o = 60 torr.						
82 BIG/CLA ¹⁾	EX	651	1.2(-2)			1
P(Total) _o = (43-161) torr.						
¹⁾ Pyrolysis in a flow-system. Other k's, at various pressures, with added Cyclohexane, also given.						
$\text{CH}_3\text{C(O)C(O)CH}_3 \rightarrow \text{CH}_3\text{CO} + \text{CH}_3\text{CO}$ (a)						
\rightarrow any other products (b)						
2,3-Butanedione						
73 KNO/SCH ¹⁾	EX	240-277	3.16(16)	0	34071±2214	1 25.1
75 SCH/PLA ¹⁾	EX	822-905	6.31(15)	0	33619±856	1 3.16
¹⁾ k _a .						
73 KNO/SCH ²⁾	EX	240-277	1.58(17)	0	33920±1158	1 5.01
75 SCH/PLA ²⁾	EX	822-905	3.98(13)	0	28083±2114	1 10.0
75 SCH/PLA ²⁾	EX	822-905	1.26(15)	0	31454±2365	1 12.59
Inhibited by Toluene.						
²⁾ k _{overall} .						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CO} \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2 + \text{CO}$						
Butyl, 1-oxo-						
79 FOE/BER	DE	273-426	1.0(15)	0	5291±302	1 2.51
Butanal photolysis. k estimated on the basis of a suggested reaction scheme.						
$\text{CH}_2\text{CH}_2\text{C(O)CH}_3 \rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CO}$						
Butyl, 3-oxo-						
75 KNO/SCH	RL	515-712	1.26(2)	0	8153±403	1/2
k _{ref} : $\text{CH}_2\text{CH}_2\text{COCH}_3 + \text{CH}_3\text{COCH}_2\text{CH}_2\text{COCH}_3$ $\rightarrow \text{CH}_3\text{COCH}_2\text{CH}_3 + \text{CH}_2\text{COCH}_2\text{CH}_2\text{COCH}_3$ (a) $\rightarrow \text{CH}_3\text{COCH}_2\text{CH}_3 + \text{CH}_3\text{COCHCH}_2\text{COCH}_3$ (b)						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

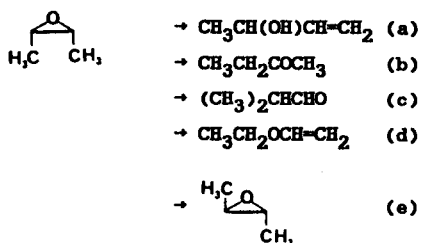
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃CH₂CHCHO → CH₃ + CH₂=CHCHO						
Propyl, 1-formyl-						
79 FOE/BER ¹⁾	RL	426	1.26(-11)			1/2
79 FOE/BER ¹⁾	RL	529	2.51(-10)			1/2
k_{ref} :						
$\begin{aligned} & \text{H}_3\text{CH}_2\text{CHCHO} + \text{CH}_3\text{CH}_2\text{CH}_2 \\ & \quad \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_2\text{CH}_3)\text{CHO} \end{aligned}$						
k/k _{ref} ratios estimated on the basis of a suggested reaction scheme.						
(CH₃)₂CCHO (+ M) → CH₃CH=CH₂ + CHO (+ M)						
Ethyl, 1,1-dimethyl-2-oxo-						
79 BAL/CLE	RL	713	(1.4±0.2)(-2)			2/2
Oxidation in an aged boric-acid-coated vessel.						
P(Total) = 60 torr.						
k_{ref} :						
$(\text{CH}_3)_2\text{CCHO} + \text{O}_2 \rightarrow (\text{CH}_3)_2\text{CO} + \text{CO} + \text{OH}$						
CH₃CH(OH)CH=CH₂ → CH₃ + CH(OH)CH=CH₂ (a)						
→ CH₂=CHCH=CH₂ + H₂O (b)						
3-Buten-2-ol						
73 TRE ¹⁾	EX	773-834	1.82(16)	0	34826±302	1 3.16
k_a .						
73 TRE ¹⁾	EX	773-834	7.94(12)	0	28032±805	1 3.16
k_b .						
¹⁾ Pyrolysis in a static reactor.						
CH₃OCH₂CH=CH₂ → HCHO + CH₃CH=CH₂						
1-Propene, 3-methoxy-						
77 IBU/TAK	EX	287	1.11(8)			1
CH₃CH₂OCH=CH₂ → CH₃CHO + CH₂CH₂						
Ethene, ethoxy-						
79 ROS/GOL	EX	750-1050	2.95(11)	0	21842±503	1 1.78
VLP-Pyrolysis.						
RRKM best-fit.						
High-pressure k.						
CH₃CH₂C(O)CH₃ (+ M) → CH₃CH₂ + CH₃CO (+ M)						
2-Butanone						
75 ABU/LIS	EX	291-346	4.27(14)	0	6397±1082	1 30.9
M = CH ₃ CH ₂ CH ₃ .						
Limiting high-pressure k.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 \rightarrow cis-CH ₃ CH=CHCH ₂ OH (a) \rightarrow trans-CH ₃ CH=CHCH ₂ OH (b) \rightarrow CH ₃ CH ₂ CH ₂ CHO (c) \rightarrow CH ₃ CH ₂ COCH ₃ (d) \rightarrow cis-CH ₃ OCH=CHCH ₃ (e) \rightarrow trans-CH ₃ OCH=CHCH ₃ (f)							
Oxirane, ethyl-							
\rightarrow 2-Buten-1-ol, (Z)-	(a)						
\rightarrow 2-Buten-1-ol, (E)-	(b)						
\rightarrow Butanal	(c)						
\rightarrow 2-Butanone	(d)						
\rightarrow 1-Propene, 1-methoxy, (Z)-	(e)						
\rightarrow 1-Propene, 1-methoxy, (E)-	(f)						
75 FLO/PEN ¹⁾ k _a + k _b . Uncertainty of A is 1318.	EX	674-730	7.76(10)	0	25741±5028	1	
75 FLO/PEN ¹⁾ k _c .	EX	674-730	8.91(13)	0	28676±662	1	2.57
75 FLO/PEN ¹⁾ k _d .	EX	674-730	1.32(14)	0	29915±1263	1	6.03
75 FLO/PEN ¹⁾ k _e + k _f .	EX	674-730	1.62(12)	0	27317±1202	1	5.62
¹⁾ Thermolysis. Static system. Gas-chromatography. Mass-spectrometry. P = (5-70) torr.							
 \rightarrow (CH ₃) ₂ CHCHO (a) \rightarrow CH ₂ =C(CH ₃)OCH ₃ (b) \rightarrow CH ₂ =C(CH ₃)CH ₂ OH (c)							
Oxirane, 2,2-dimethyl-							
\rightarrow 2-Propanal, 2-methyl-	(a)						
\rightarrow 1-Propene, 2-methoxy-	(b)						
\rightarrow 2-Propen-1-ol, 2-methyl-	(c)						
71 FLO/PAR1 ¹⁾ k _a .	EX	647-705	2.09(13)	0	26532±287	1	1.51
71 FLO/PAR1 ¹⁾ k _b .	EX	647-705	3.55(13)	0	28254±735	1	2.75
71 FLO/PAR1 ¹⁾ k _c .	EX	647-705	3.39(11)	0	25003±1047	1	4.68
¹⁾ Pyrolysis in a static system. Gas-chromatography.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
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Oxirane, 2,3-dimethyl- cis- (cis-2,3-Epoxybutane)

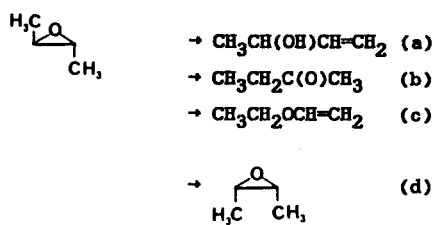
- \rightarrow 3-Buten-2-ol (a)
- \rightarrow 2-Butanone (b)
- \rightarrow 2-Propanal, 2-methyl- Isobutyraldehyde (c)
- \rightarrow Ethene, ethoxy- (Ethyl vinyl ether) (d)
- \rightarrow Oxirane, 2,3-dimethyl-, trans-
(trans-2,3-Epoxybutane) (e)

71 FLO/PAR2 ¹⁾	EX	668-740	1.51(12)	0	27172±1505	1	8.71
k_a . Decyclization.							
71 FLO/PAR2 ¹⁾	EX	668-740	3.98(13)	0	28344±332	1	1.62
k_b . Decyclization.							
71 FLO/PAR2 ¹⁾	EX	668-740	9.77(12)	0	28168±991	1	4.17
k_c . Decyclization.							
71 FLO/PAR2 ¹⁾	EX	668-740	8.71(12)	0	27796±1530	1	9.12
k_d . Decyclization.							
71 FLO/PAR2 ¹⁾	EX	668-740	3.89(14)	0	31117±846	1	3.39
k_e . Cis-trans isomerization.							

¹⁾ Thermolysis. Static system.

Gas-chromatography. Mass-spectrometry.

$P_0 = 22$ torr.




Oxirane, 2,3-dimethyl- trans- (trans-2,3-Epoxybutane)

- \rightarrow 3-Buten-2-ol (a)
- \rightarrow 2-Butanone (b)
- \rightarrow Ethene, ethoxy- (Ethyl vinyl ether) (c)
- \rightarrow Oxirane, 2,3-dimethyl-, cis-
(cis-2,3-Epoxybutane) (d)

71 FLO/PAR2 ¹⁾	EX	668-740	5.37(12)	0	28007±1309	1	6.45
k_a . Decyclization.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
71 FLO/PAR2 ¹⁾ k _b . Decyclization.	EX	668-740	1.74(14)	0	29839±1067	1	4.47
71 FLO/PAR2 ¹⁾ k _c . Decyclization.	EX	668-740	1.70(14)	0	31595±1228	1	5.62
71 FLO/PAR2 ¹⁾ k _d . Trans-cis isomerization.	EX	668-740	4.68(14)	0	31711±8800	1	3.09
¹⁾ Thermolysis. Static system. Gas-chromatography. Mass-spectrometry. Mass-spectrometry. P _o = 22 torr.							
							
→ HCHO + CH ₃ CH=CH ₂ (a)							
→ CH ₃ CHO + CH ₂ =CH ₂ (b)							
Oxetane, 2-methyl-							
82 HAM/HOL k _a + k _b . Pyrolysis in a cylindrical Pyrex vessel with vacuum system. Gas-chromatography. P = (6.0-1.42) torr.	EX	703-756	7.76(14)	0	30047±565	1	2.29
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OH} + \text{CH}_2=\text{CH}_2$							
Acetic acid ethyl ester (Ethyl acetate)							
72 BEA/GOL2 VLPP of Ethyl acetate in Ar, in a triple aperture quartz reactor. Gas-chromatography. Mass-spectrometry. The data agree well with the high-P Arrhenius expression determined by Blades and Gilderson, Can. J. Chem. 38, 1407 (1960).	EX	772-1156	3.98(12)	0	24157	1	
75 TAY Pyrolysis. Acetic acid decomposes further into CO ₂ + CH ₄ in a fast reaction.	EX	650-700	3.16(12)	0	24056±503	1	2.0
76 DEB/TAY	EX	650-700	3.16(12)	0	24006	1	
82 KEL/FET Thermolysis in a flow-reactor. P = 750 torr.	EX	940-1050	3.92(12)	0	24538	1	
82 MCM/LEW ¹⁾ k determined versus Isobutyl bromide.	RN	950-1000	5.0(12)	0	24912	1	
82 MCM/LEW ¹⁾ k determined versus Isopropyl acetate.	RN	950-1000	6.31(12)	0	24660	1	
¹⁾ Laser-powered homogeneous pyrolysis of an Ethyl acetate/Isopropyl acetate/Isobutyl bromide/SF ₆ /CO ₂ mixture. Gas-chromatography. P(Acetate, or Bromide) ~ 1.0 torr. P(SF ₆) = 4 torr. P(CO ₂) = 93 torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{OC}(\text{O})\text{OCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$ Carbonic acid ethyl methyl ester						
76 CRO/HUN	EX	581-667	5.25(11)	0	21892	1
$\text{CH}_3\text{CH}(\text{OH})\text{CHCH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{CH}(\text{OH})\text{CH}(\text{O}_2)\text{CH}_3$ Propyl, 2-hydroxy-1-methyl- + Oxygen molecule						
80 LEN/MCD M = He. 3-Iodo-2-butanol flash-photolysis. Photoionization Mass-spectrometer. Limiting high-pressure k. P-independent for (1-4) torr.	EX	298	(1.69±1.08)(13)			2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ Butoxy						
80 ROS Butyl nitrite/ NO_2 photolysis at 366 nm. $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} + \text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{ONO}_2$	RL	298	(2.8±0.5)(-8)			1/2
81 COX/PAT HONO/ N_2/O_2 /Butane photolysis. P = 760 torr. $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{O} + \text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CHO} + \text{HO}_2$	RL	296	(2.49±0.83)(-5)			1/2
$\text{CH}_3\text{CH}_2\text{CH}(\text{O}\cdot)\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CHO}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CHO} + \text{CH}_3$ (b) Propoxy, 1-methyl-						
75 BAT/MCC ¹⁾	ES	393-473	1.0(16)	0	8807	1
76 BAT/MCC2 ¹⁾	ES	403-433	6.31(14)	0	7700	1
79 BAT ¹⁾ Static system.	ES	403-433	7.94(14)	0	7700±503	1 3.16
81 COX/PAT ¹⁾ HONO/ N_2/O_2 /Butane photolysis. P = 760 torr. $k_{\text{ref}}: \text{CH}_3\text{CH}_2\text{CH}(\text{O}\cdot)\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{HO}_2$ ¹⁾ k_a .	RL	296	(4.32±0.58)(-6)			1/2
79 BAT k_b . Static system.	ES	403-433	7.9(14)	0	9562	1
$\text{CH}_3\text{CH}_2\text{CH}(\text{O}\cdot)\text{CH}_3 + \text{NO} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{HNO}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{ONO}$ (b) Propoxy, 1-methyl- + Nitrogen oxide (NO)						
75 BAT/MCC ¹⁾	ES	393-473	3.98(12)	0	0±503	2 3.16
76 BAT/MCC2 ¹⁾ ¹⁾ k_a .	ES	403-433	6.31(12)	0	0±503	2 2.51
76 BAT/MCC2 k_b . Same data given in 75 BAT/MCC.	ES	403-433	2.51(13)	0	0±503	2 2.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{CH}(\text{O}\cdot)\text{CH}_3 + \text{NO}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{HONO}$ (a)						
$\rightarrow \text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{ONO}_2$ (b)						
Propoxy, 1-methyl- + Nitrogen oxide (NO_2)						
80 ROS	RL	298	(8.0±8.0)(-2)			2/2
k_a/k_b . sec-Butyl nitrite/ NO_2 photolysis at 366 nm. Gas-chromatography.						
$(\text{CH}_3)_3\text{CO} \rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3$						
Ethoxy, 1,1-dimethyl- (t-Butoxy)						
71 CAD/TRO	EX	373-423	2.34(13)	0	8444±746	1 6.61
Limiting high-pressure k.						
75 BAT/MCC	ES	393-473	3.98(15)	0	8606	1
76 BAT/MIL	ES	393-433	4.0(15)	0	8556	1
79 BAT	ES	393-433	3.16(15)	0	8556±503	1 3.16
Static system.						
81 CHO/BEN	RE	248-450	1.26(14)	0	7700	1
Recommended by the authors.						
Critical evaluation.						
81 KIR/PAR ¹⁾	RL	298	5.0(14)			1/2
81 KIR/PAR ¹⁾	RL	333	1.0(16)			1/2
¹⁾ Azo-t-butane/ O_2 photolysis. Gas-chromatography. Approximate rate ratios.						
k_{ref} :						
$(\text{CH}_3)_3\text{CO} + (\text{CH}_3)_3\text{COOH} \rightarrow (\text{CH}_3)_3\text{COH} + (\text{CH}_3)_3\text{CO}_2$						
82 BAT/ROB ²⁾	EX	403-443	3.98(14)	0	8002±604	1 3.98
82 BAT/ROB ²⁾	CO	403-443	7.94(14)	0	8354	1
RRKM best-fit.						
²⁾ M = CF_4 , SF_6 , N_2 , Ar.						
Limiting high-pressure k. Static system.						
$(\text{CH}_3)_3\text{C}$ decomposition in presence of NO and an inert gas. $(\text{CH}_3)_3\text{C}$ generated by decomposition of di-t-Butyl peroxide.						
P[inert gas] = (25-1500) torr.						
$(\text{CH}_3)_3\text{CO} + \text{NO} \rightarrow (\text{CH}_3)_3\text{CONO}$						
Ethoxy, 1,1-dimethyl- (t-Butoxy) + Nitrogen oxide (NO)						
74 BAT/MIL	ES	393-473	2.51(13)	0	0±503	2 2.51
75 BAT/MCC	ES	393-473	2.51(13)	0	0±503	2 2.51
75 MEN/GOL	DE	300	6.31(12)	0	0	2
B ~ 0 assumed. Estimated k.						
77 BAR/BEN2	ES	650-800	6.31(12)			2
VLP-Pyrolysis.						
RRKM best-fit estimate.						

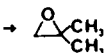
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
(CH₃)₃CO + HCHO → (CH₃)₃COH + CHO							
Ethoxy, 1,1-dimethyl- (t-Butoxy) + Formaldehyde							
81 ALA/SEL ¹)	RN	399-434	7.94(12)	0	2322±277	2	1.58
Calculated by using: logA _{ref} = 17.5(c ³ mol ⁻¹ s ⁻¹).							
81 ALA/SEL ¹)	RN	399-434	1.58(13)	0	1985±265	2	1.58
Calculated by using: logA _{ref} = 18.5(c ³ mol ⁻¹ s ⁻¹).							
¹) Cylindrical Pyrex vessel. Static system.							
(CH ₃) ₃ CO generated by thermolysis of							
Di-t-butyl peroxide. Mass-spectrometry.							
P(Total) = (20-200) torr.							
k _{ref} : (CH ₃) ₃ O + M → CH ₃ + (CH ₃) ₂ CO + M.							
(CH₃)₃CO + CH₃CHO → (CH₃)₃COH + CH₂CHO (a)							
→ (CH₃)₃COH + CH₃CO (b)							
Ethoxy, 1,1-dimethyl- (t-Butoxy) + Acetaldehyde							
81 ALA/SEL ¹)	RN	399	(1.1±0.1)(10)			2	
k _a + k _b . Sum of rate constants determined relative to the reaction:							
(CH ₃) ₃ CO + M → CH ₃ + (CH ₃) ₂ CO + M							
81 ALA/SEL ¹)	RN	434	(1.6±0.1)(10)			2	
k _a + k _b . Sum of rate constants determined relative to the reaction:							
(CH ₃) ₃ CO + M → CH ₃ + (CH ₃) ₂ CO + M							
81 ALA/SEL ¹)	RL	399	(4.7±0.8)(-2)			2/2	
k _a /k _b . Estimated ratio.							
81 ALA/SEL ¹)	ES	399	(4.9±1.5)(8)			2	
k _a .							
81 ALA/SEL ¹)	ES	434	(7.2±0.2)(8)			2	
k _a .							
81 ALA/SEL ¹)	ES	399	(1.0±0.7)(10)			2	
k _b .							
81 ALA/SEL ¹)	ES	434	(1.5±0.6)(10)			2	
k _b .							
¹) Cylindrical Pyrex vessel. Static system.							
(CH ₃) ₃ CO generated by thermolysis of							
Di-t-butyl peroxide. Mass-spectrometry.							
(CH₃)₃CO + CD₃CHO → (CH₃)₃COD + CD₂CHO (a)							
→ (CH₃)₃COH + CD₃CO (b)							
Ethoxy, 1,1-dimethyl- (t-Butoxy)							
+ Acetaldehyde-2,2,2-d ₃							
81 ALA/SEL ¹)	RL	399	(1.0±0.2)(-2)			2/2	
k _a /k _b .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
81 ALA/SEL ¹) k _a . Estimated k. ¹) Pyrex vessel with vacuum system. (CH ₃) ₃ CO generated by thermolysis of Di-t-butyl peroxide. Mass-spectrometry.	RN	399	(1.1±0.3)(8)			2
(CH ₃) ₃ CO + (CH ₃) ₂ CO → (CH ₃) ₃ COH + CH ₂ C(O)CH ₃ Ethoxy, 1,1-dimethyl- (t-Butoxy) + 2-Propanone						
81 ALA/SEL ¹) Calculated by using: logA _{ref} = 17.5(c ³ mol ⁻¹ s ⁻¹).	RN	399-434	1.26(13)	0	3091±156	2 1.26
81 ALA/SEL ¹) Calculated by using: logA _{ref} = 18.5(c ³ mol ⁻¹ s ⁻¹).	RN	399-434	3.16(13)	0	2874±397	2 2.0
¹) Di-tert-butyl peroxide thermolysis in a Pyrex vessel with vacuum system. Mass-spectrometry. k _{ref} : (CH ₃) ₃ CO + M → CH ₃ + (CH ₃) ₂ CO + M.						
(CH ₃) ₃ CO + (CD ₃) ₂ CO → (CH ₃) ₃ COD + CD ₂ C(O)CD ₃ Ethoxy, 1,1-dimethyl- (t-Butoxy) + 2-Propanone-1,1,1,3,3,3-d ₆						
81 ALA/SEL ¹) Calculated by using: logA _{ref} = 17.5(c ³ mol ⁻¹ s ⁻¹).	RN	399-434	1.58(13)	0	3801±361	2 1.58
81 ALA/SEL ¹) Calculated by using: logA _{ref} = 18.5(c ³ mol ⁻¹ s ⁻¹).	RN	399-434	2.00(13)	0	3271±337	2 2.0
¹) Di-tert-butyl peroxide thermolysis in a Pyrex vessel with vacuum system. Mass-spectrometry. k _{ref} : (CH ₃) ₃ O + M → CH ₃ + (CH ₃) ₂ CO + M.						
(CH ₃) ₃ CO + (CH ₃) ₃ CH → (CH ₃) ₃ COH + (CH ₃) ₃ C Ethoxy, 1,1-dimethyl- (t-Butoxy) + Propane, 2-methyl- (Isobutane)						
82 PAR/SON Reaction in a static-photolysis reactor. (CH ₃) ₃ CO generated by UV-photolysis of Di-t-butyl peroxide. k determined relative to the reaction: (CH ₃) ₃ CO → CH ₃ + (CH ₃) ₂ CO	RN	316-338	2.51(11)	0	2164	2 3.16
(CH ₃) ₃ CO ₂ + NO → products Ethyldioxy, 1,1-dimethyl- + Nitrogen oxide (NO)						
78 ANA/SMI2 Azoisobutane/O ₂ /NO ₂ flash-photolysis. [Azoisobutane] = (1.0-3.0)x10 ¹⁷ molec.cm ⁻³ . [NO] = (0.1-1.0)x10 ¹⁶ molec.cm ⁻³ . Lower-limit k.	EX	298	>6.02(11)			2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
(CH₃)₃CO₂ + NO₂ → products						
Ethyldioxy, 1,1-dimethyl- + Nitrogen oxide (NO ₂)						
78 ANA/SMI2 Azoisobutane/O ₂ /NO ₂ flash-photolysis. [Azoisobutane] = (1-3)x10 ¹⁷ molec.cm ⁻³ . Lower-limit k.	EX	298	>3.01(11)			2
(CH₃)₃CO₂ + (CH₃)₃CO₂ → (CH₃)₃CO + (CH₃)₃CO + O₂ (a) → (CH₃)₃COOC(CH₃)₃ + O₂ (b)						
Ethyldioxy, 1,1-dimethyl-						
75 PAR k _a . Unreported T assumed to be 298 K.	EX	298	(2.17±0.48)(6)			2
81 KIR/PAR ¹⁾	RL	298	1.4(-1)			2/2
81 KIR/PAR ¹⁾	RL	333	5.0(-2)			2/2
¹⁾ k _b /k _a . Azo-t-butane/O ₂ photolysis. Approximate rate ratios. Gas-chromatography.						
78 ANA/SMI2 k _{overall} . Azoisobutane/O ₂ flash-photolysis. [Azoisobutane] = (1-3)x10 ¹⁷ molec.cm ³ .	EX	298	(1.57±0.47)(7)			2
(CH₃)₂CCH₂OOH → CH₂=C(CH₃)CH₂OH + OH (a) → CH₂=C(CH₃)CHO + OH + H₂ (b) → (CH₃)₂CHCHO + OH (c) →  + OH (d)						
Ethyl, 1-(hydroperoxymethyl)-1-methyl-						
→ 2-Propen-1-ol, 2-methyl- + Hydroxyl (a)						
→ 2-Propenal, 2-methyl- (Methacrolein) + Hydroxyl + Hydrogen molecule (b)						
→ Propanal, 2-methyl- + Hydroxyl (c)						
→ Oxirane, 2,2-dimethyl- + Hydroxyl (d)						
78 BAK/BAL ¹⁾ k _a .	ES	753	1.3(5)			1 2.0
78 BAK/BAL ¹⁾ k _b .	ES	753	1.3(5)			1 2.0
78 BAK/BAL ¹⁾ k _c .	ES	753	4.2(5)			1 2.0
78 BAK/BAL ¹⁾ k _d .	ES	753	1.8(6)			1 2.0
¹⁾ Aged boric-acid-coated vessels. P(Total) = (490-505) torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CHCH}_2\text{O}_2 \rightarrow (\text{CH}_3)_2\text{CCH}_2\text{OOH}$ (a) $\rightarrow \text{CH}_3\text{CH}(\text{CH}_2\text{OOH})\text{CH}_2$ (b)						
Propyldioxy, 2-methyl-						
78 BAK/BAL ¹⁾ k_a/k_b	RL	753	(4.08±0.41)			1/1
78 BAK/BAL ¹⁾ k_a	RN	753	1.8(5)			1
78 BAK/BAL ¹⁾ k_b	RN	753	4.5(4)			1
¹⁾ Aged boric-acid-coated vessels. Rate constants computed by Benson's group additivity method. P(Total) = (490-505) torr.						
$(\text{CH}_3)_2\text{C}(\text{OO}\cdot)\text{CH}_2\text{OOH} \rightarrow (\text{CH}_3)_2\text{CO} + \text{HCHO} + \text{HO}_2$						
Ethyldioxy, 1-(hydroperoxymethyl)-1-methyl-						
78 BAK/BAL	ES	753	2.5(6)			1 2.0
Aged boric-acid-coated vessels. P(Total) = (490-505) torr.						
$(\text{CH}_3)_3\text{COH} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{H}_2\text{O}$ (a) $\rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{C}(\text{OH})$ (b)						
2-Propanol, 2-methyl- (t-Butanol)						
71 GON/LEW ¹⁾	EX	753-833	2.50(5)	0	15136	1
71 DOR/MCG ¹⁾ Pyrolysis. M = He + Ar. Reflected shock-waves.	EX	935-1397	2.24(13)	0	30448±50	1 1.58
74 LEW/KEI ¹⁾ Pyrolysis. M = He + Ar. Reflected shock-waves. P = (370-1560) torr.	EX	920-1175	3.98(14)	0	33317±503	1 1.58
¹⁾ k_a						
76 TSA1 k_b	ES	1080-1165	6.31(16)	0	40900	1
$(\text{CH}_3\text{CH}_2)_2\text{O} \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2\text{O}$						
Ethane, 1,1'-oxybis- (Diethyl ether)						
77 SER/LAB Thermolysis.	ES	763-823	5.0(15)	0	40765	1


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃SCH₂CH=CH₂ → HC₂S + CH₃CH=CH₂						
1-Propene, 3-(methylthio)- → Methanethial + 1-Propene						
82 MAR/ROP2 Pyrolysis in a stirred-flow system. Gas-chromatography. Mass-spectrometry. P = (2-15) torr. HC ₂ S polymerizes, to give probably the cyclic trimer 1,3,5-Trithiane.	EX	588-691	1.70(11)	0	19426±361	1 1.78
CH₃C(S)SCH₂CH₃ → CH₄ + CS₂ + CH₂=CH₂						
Ethane(dithioic) acid ethyl ester						
78 ALA/BIG ¹⁾	EX	629	1.80(-3)			1
78 ALA/BIG ¹⁾	EX	651-716	8.83(12)	0	22725	1
A and B recalculated from the reported data. ¹⁾ Pyrolysis in a flow-reactor. Gas-chromatography. IR-, and NMR-spectrometry.						
CH₃C(O)SCH₂CH₃ → CH₄ + COS + CH₂=CH₂						
Ethanethioic acid S-ethyl ester						
72 OEL/TIN Elimination by thermolysis.	EX	763-841	2.51(12)	0	25365	1
CH₃C(S)OCH₂CH₃ → CH₄ + COS + CH₂=CH₂ (a) → CH₃C(O)SCH₂CH₃ (b)						
Ethanethioic acid O-ethyl ester						
72 OEL/TIN k _a . Elimination by thermolysis. Channel (a) is predominant. T-range assumed to be the same as that of Ethanedithioic acid S-ethyl ester (see above).	EX	763-841	3.16(12)	0	20735	1
75 BIG/GAB ¹⁾ k _a . Elimination.	EX	629	1.15(-2)			1
75 BIG/GAB ¹⁾ k _b . Isomerization.	EX	629	1.73(-3)			1
75 BIG/GAB ¹⁾ k _a + k _b . Overall reaction.	EX	635	1.78(-2)			1
75 BIG/GAB ¹⁾ k _a + k _b . Overall reaction.	EX	625-653	3.55(12)	0	20886	1
¹⁾ Flow reactor pyrolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
CH₃OC(S)OCH₂CH₃ → CH₃OH + COS + CH₂=CH₂						
Carbonothioic acid O-ethyl O-methyl ester						
82 ALA/BIG ¹⁾	EX	629	1.3(-2)			1
82 ALA/BIG ¹⁾	EX	570-660	3.22(10)	0	17950	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow reactor.						
IR-spectrometry.						
P = (2-800) torr.						
CH₃OC(O)SCH₂CH₃ → CH₃OH + COS + CH₂=CH₂						
Carbonothioic acid S-ethyl O-methyl ester						
79 ALA/BIG ¹⁾	EX	629	7.75(-7)			1
79 ALA/BIG ¹⁾	EX	763-823	1.24(13)	0	27813±722	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow-reactor.						
Flow-tube method.						
IR-spectrometry.						
CH₃CH₂OC(O)SCH₃ → CH₂=CH₂ + CO₂ + CH₃SH						
Carbonothioic acid O-ethyl S-methyl ester						
79 ALA/BIG ¹⁾	EX	7629	1.0(-4)			1
79 ALA/BIG ¹⁾	EX	763-823	1.64(12)	0	23483±721	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow-reactor.						
Flow-tube method.						
IR-spectrometry.						
CH₃SC(S)OCH₂CH₃ → CH₃SH + COS + CH₂=CH₂						
Carbonodithioic acid O-ethyl S-methyl ester						
82 ALA/BIG ¹⁾	EX	629	1.4(-2)			1
82 ALA/BIG ¹⁾	EX	590-620	8.95(11)	0	19995	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow reactor.						
IR-spectrometry.						
P = (2-800) torr.						
CH₂=CHCH₂NC → CH₂=CHCH₂CN						
1-Propene, 3-isocyano-						
79 GLI/PRI	EX	403-493	5.89(14)	0	20533±302	1 2.0
Thermal isomerization in a Pyrex bulb.						
Gas-chromatography.						
P = 20 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
cis-CH₃CH=CHCN → trans-CH₃CH=CHCN							
2-Butenenitrile, (Z)- (cis-Crotononitrile)							
→ 2-Butenenitrile, (E)-							
75 MAR/JEF	EX	1060-1380	1.58(13)	0	29190±1007	1	2.0
M = Ar. Single-pulse shock-tube isomerization.							
Limiting high-pressure k.							
P(Ar) = (200-340) torr.							
	→ cis-CH ₃ CH=CHCN (a)						
	→ trans-CH ₃ CH=CHCN (b)						
	→ CH ₂ =CHCH ₂ CN (c)						
Cyclopropanecarbonitrile (Cyclopropyl cyanide)							
→ 2-Butenenitrile, (Z)- (cis-Crotononitrile) (a)							
→ 2-Butenenitrile, (E)- (trans-Crotononitrile) (b)							
→ 3-Butenenitrile (Allyl cyanide) (c)							
73 LUC/ROB ¹⁾	EX	660-760	1.02(14)	0	28580±168	1	1.29
k _a .							
73 LUC/ROB ¹⁾	EX	660-760	1.23(14)	0	29313±108	1	1.17
k _b .							
73 LUC/ROB ¹⁾	EX	660-760	3.89(14)	0	30372±217	1	1.35
k _c .							
73 LUC/ROB ¹⁾	EX	660-760	3.80(14)	0	29109±144	1	1.20
k _a + k _b + k _c .							
¹⁾ Thermal isomerization in a silica reaction vessel with Pyrex vacuum system.							
Gas-chromatography.							
CH₃CH₂CH₂CN → CH₃CH₂ + CH₂CN							
Butanenitrile							
75 KIN/GOD2	EX	1090-2050	2.51(15)	0	38601±856	1	2.0
(CH₃)₂CHCN → CH₃CH=CH₂ + HCN (a)							
→ CH₃CHCN + CH₃ (b)							
Propanenitrile, 2-methyl-							
73 DAS/EMO	EX	820-928	1.58(12)	0	32280±523	1	1.12
k _a .							
75 KIN/GOD1	EX	1074-1253	7.94(13)	0	38349±1007	1	2.0
k _a .							
75 KIN/GOD1	EX	1074-1250	5.01(15)	0	39758±1007	1	2.0
k _b .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{CHCH}_2\text{NHCH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_2=\text{NH}$							
2-Propen-1-amine, N-methyl- (N-Allyl-N-methylamine)- → 1-Propene + Methanimine							
74 VIT/EGG2 Pyrolysis in a static system. Gas-chromatography. P(CH ₂ =CHCH ₂ NHCH ₃) = (9-71) torr.	EX	602-694	2.34(11)	0	21832±815	1	3.63
$\text{CH}_3\text{N}=\text{NCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_2\text{CH}=\text{CH}_2 + \text{N}_2$							
Diazene, methyl-(2-propenyl)-							
72 CRA/TAK ¹⁾ k _{ref} : CH ₃ N=NCD ₂ CH=CH ₂ → CH ₃ + CD ₂ CH=CH ₂ + N ₂	RL	399	(1.28±0.05)			1/1	
72 CRA/TAK ¹⁾ Uninhibited k.	EX	436-456	3.24(14)	0	17816±352	1	2.09
72 CRA/TAK ¹⁾ In presence of ¹⁵ NO.	EX	383-403	2.29(14)	0	17866±352	1	2.40
¹⁾ Thermolysis. Mass-spectrometry. Gas-chromatography. P(Total) = (50-60) torr.							
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 + \text{N}_2$							
Diazene, diethyl- (Azoethane)							
73 PER/BEA RRKM fit of experimental data.	EX	700-950	2.51(16)	0	25013±503	1	
77 MAR/MAC ¹⁾	EX	553-673	1.58(14)	0	22373±241	1	1.58
80 ACS/PET ¹⁾	EX	523-623	6.31(15)	0	24670±180	1	1.26
¹⁾ Azoethane thermolysis in a vacuum system.							
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_3^* \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}_2 + \text{N}_2$							
Diazene, diethyl- (Azoethane)							
77 CHE/ORE High-pressure photolysis of Azoethane in He. RRKM data fit on the basis of a proposed mechanism. Azoethane is assumed to be in a vibrationally excited T ₁ electronic state. Lower-limit k. P(He) = (0-150) atm. P(CO ₂) = (0-45) atm.	EX	298	6.0(9)			1	
$(\text{CH}_3)_2\text{NN}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{N} + (\text{CH}_3)_2\text{N}$							
Hydrazine, tetramethyl-							
72 GOL/SOL RRKM fit of experimental data.	EX	720-930	2.51(17)	0	27177	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
NCC(O)OCH₂CH₃ → HCN + CO₂ + CH₂=CH₂							
Carbonocyanidic acid ethyl ester (Ethyl cyanoformate)							
74 BAR/DES Thermolysis.	EX	613-678	2.75(11)	0	21439±307	1	1.78
(CH₃)₃CNO → (CH₃)C + NO							
Propane, 2-methyl-2-nitroso-							
74 CHO/MEN	EX	550-850	3.98(15)	0	18118±503	1	3.2
CH₃CH₂CH₂CH₂ONO → CH₃CH₂CH₂CH₂O + NO							
Nitrous acid butyl ester (n-Butyl nitrite)							
78 BAL/GOL VLP-Pyrolysis. Best RRKM data-fit.	EX	590-750	3.16(16)	0	20634	1	
CH₃CH₂CH(CH₃)ONO → CH₃CH₂COCH₃ + HONO (a) → CH₃CH₂CH(O·)CH₃ + NO (b)							
Nitrous acid 1-methylpropyl ester (s-Butyl nitrite)							
76 BAT/MCC2 k _a .	EX	403-433	6.31(12)	0	18017±403	1	3.16
75 BAT/MCC k _b .	EX	393-473	1.26(16)	0	20735±403	1	2.51
76 BAT/MCC2 k _b .	EX	403-433	1.58(16)	0	20584±403	1	2.51
76 BAT/MCC2 k _a + k _b .	EX	403-433	5.01(15)	0	19926±403	1	3.16
(CH₃)₃CONO → (CH₃)₂C=CH₂ + HONO (a) → (CH₃)₃CO + NO (b)							
Nitrous acid 1,1-dimethylethyl ester (t-Butyl nitrite)							
76 BAT/MIL k _a . Same data given in 74 BAT/MIL and 75 BAT/MCC.	EX	393-433	7.9(12)	0	16910±403	1	2.51
75 MEN/GOL k _b . RRKM fit of experimental data.	CO	300	6.31(15)	0	19779	1	
76 BAT/MIL k _b . Same data given in 74 BAT/MIL and 75 BAT/MCC.	EX	393-433	2.0(16)	0	20282±403	1	2.51

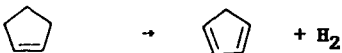
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 BAR/BEN2 k_b . VLP-Pyrolysis. RRKM best-fit estimate.	ES	650-800	6.31(15)	0	19779	1
76 BAT/MIL $k_a + k_b$. Same data given in 74 BAT/MIL and 75BAT/MCC.	EX	393-433	5.0(14)	0	18218±403	1 2.51
$(CH_3)_3CONO_2 \rightarrow (CH_3)_3CO + NO_2$ Nitric acid 1,1-dimethylethyl ester (t-Butyl nitrate)						
76 BAT/MIL	ES	393-433	7.9(15)	0	20232	1
$(CH_3CH_2)_2NO + NO_2 \rightarrow CH_3CH_2N(\uparrow O)=CHCH_3 + HONO$ Nitroxide, diethyl- + Nitrogen oxide (NO_2)						
82 GLE/HEI Oxidation of Diethylhydroxylamine by NO_2 in a variable path-length IR gas-cell. IR-Spectrometry. [(CH_3CH_2) ₂ NOH] = (25-45) mtorr. [CH_3CHO] = (0-32) mtorr. [NO_2] = (15-236) mtorr. [HONO] = (11-15) mtorr.	ES	298	≈1.51(6)			2
$(CH_3CH_2)_2NOH + NO_2 \rightarrow (CH_3CH_2)_2NO + HONO$ (a) Ethanamine, N-ethyl-N-hydroxy- + Nitrogen oxide (NO_2)						
82 GLE/HEI k_a . Oxidation of Diethylhydroxylamine by NO_2 in a variable path-length IR gas-cell. IR-Spectrometry. [(CH_3CH_2) ₂ NOH] = (25-45) mtorr. [CH_3CHO] = (0-32) mtorr. [NO_2] = (15-236) mtorr. [HONO] = (11-15) mtorr.	ES	298	(3.31±0.60)(6)			2
74 JAY/SIM $k_{overall}$. Dark reaction of (CH_3CH_2) ₂ NOH (diluted in CO_2) with NO_2 (diluted in O_2), in a cylindrical vessel with conventional high-vacuum system. P(Diethylhydroxylamine) = 2.2 mtorr. P(NO_2) = 19.3 mtorr.	EX	298	2.71(6)			2
$(CH_3CH_2NO)_2 \rightarrow CH_3CH_2NO + CH_3CH_2NO$ Diazene, diethyl-, 1,2-dioxide- (Nitrosoethane dimer)						
72 TAN/LAM	RN	314	(4.1±0.6)(03(1

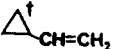


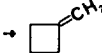
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CH₂CH₂C=CH → CH₂=CH₂ + CH₂=C=CH₂							
1-Pentyne							
81 KIN1 1-Pentyne thermolysis. VLP-Pyrolysis system. Mass-spectrometry.	EX	923-1154	6.31(12)	0	28686±1007	1	2.51
CH₃CH₂C=CCH₃ → CH₃ + CH₂C=CCH₃							
2-Pentyne							
82 NGU/KIN1 2-Pentyne thermolysis. VLP-Pyrolysis system. Mass-spectrometry. High-pressure k. 1) Curved Arrhenius plot. For 1100 K the authors give: $k = 1.0 \times 10^{16} \exp(-36537 \pm 1007) \text{ s}^{-1}$.	EX	988-1234	1)	1)	1)	1	
(CH₃)₂CHC=CH → CH₃CHC=CH + CH₃ (a) → (CH₃)₂C=C=CH₂ (b)							
1-Butyne, 3-methyl-							
81 NGU/KIN 1) k _a . Thermolysis.	EX	940-1222	2.00(16)	0	36034±503	1	2.0
81 NGU/KIN 1) k _b . Thermal isomerization.	EX	940-1222	1.58(13)	0	30448±503	1	3.98
1) Thermolysis of 3-Methyl-1-butyne in a VLP-Pyrolysis system. Mass-spectrometry.							
cis-CH₃CH=CHCH=CH₂ → CH₂=CHCH=C=CH₂ + H₂ (a) → trans-CH₃CH=CHCH=CH₂ (b)							
1,3-Pentadiene, (Z)-							
82 NGU/KIN2 k _a . cis-1,3-Pentadiene unimolecular thermolysis. VLP-Pyrolysis system. Mass-spectrometry. 1) Curved Arrhenius plot. For 1100 K the authors give: $k = 1.0 \times 10^{13} \exp(-32461 \pm 1007) \text{ s}^{-1}$.	EX	1002-1235	1)	1)	1)	1	
71 FRE/LAM k _b . Thermal isomerization in a static system. Gas-chromatography. k is P-independent between 0.75 and 75 torr. Determined from the Equilibrium constant and the sum of k _b and k _{-b} .	DE	473-517	3.09(13)	0	26210±301	1	1.55
75 MAR/JEF k _b . M = Ar. Single-pulse shock-tube Isomerization. Limiting high-pressure k. P(Ar) = (200-340) torr.	EX	1060-1280	3.98(13)	0	25673±1007	1	2.0

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{cis-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger \rightarrow \text{trans-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger$ 1,3-Pentadiene, (Z)-							
75 CRA/ROS	RL	298	(1.3±0.1)			1/1	
$\text{cis-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger$ formed by: ${}^1\text{CH}_2 + \text{CH}_2=\text{CHCH}=\text{CH}_2$							
k_{ref} : $\text{trans-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger \rightarrow \text{cis-CH}_2=\text{CHCH}=\text{CHCH}_3^\dagger$							
$\text{trans-CH}_3\text{CH}=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}=\text{C}=\text{CH}_2 + \text{H}_2$ (a) $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (b)							
1,3-Pentadiene, (E)-							
82 NGU/KIN2	EX	1002-1235	¹⁾	¹⁾	¹⁾	1	
k_a . Unimolecular thermolysis. VLPP-technique. Mass-spectrometry.							
¹⁾ Curved Arrhenius plot. For 1100 K the authors give: $k = 1.0 \times 10^{13} \exp(-32461 \pm 1007) \text{ s}^{-1}$.							
71 FRE/LAM	RN	473-517	2.00(13)	0	26487±301	1	1.55
k_b . Thermal isomerization in a static system. Gas-chromatography. k is P-independent between 0.75 and 7.5 torr. Determined from the Equilibrium constant and the sum of k_b and k_{-b} .							
$(\text{CH}_3)_2\text{C}=\text{C}=\text{CH}_2 \rightarrow \text{CH}_3\text{C}=\text{C}=\text{CH}_2 + \text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{C}=\text{CH}=\text{CH}$ (b)							
1,2-Butadiene, 3-methyl-							
81 NGU/KIN ¹⁾	EX	940-1222	2.00(16)	0	37896±53	1	2.0
k_a . Thermolysis.							
81 NGU/KIN ¹⁾	EX	940-1222	1.58(13)	0	32109±503	1	3.98
k_b . Thermal isomerization.							
¹⁾ 3-Methylbuta-1,2-diene pyrolysis in a VLP-Pyrolysis system. Mass-spectrometry.							
							
Cyclopentene							
74 LEW/SAR	EX	1020-1189	2.24(13)	0	30196±679	1	1.86
M = Ar. Thermolysis behind reflected shock-waves in a single-pulse shock-tube. [Cyclopentene] = (0.25-1.0)% in Ar. P = 760 torr.							
75 CRA/ROS	EX	298	(1.52±0.12)(8)			2	







4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 $\rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{cis-CH}_2=\text{CHCH}=\text{CHCH}_3$ (b) $\rightarrow \text{trans-CH}_2=\text{CHCH}=\text{CHCH}_3$ (c) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2$ (d) \rightarrow  (e)						
Cyclopropane, ethenyl- (Vinylcyclopropane)						
75 CRA/ROS k_a .	EX	298	(4.7±0.1)(8)			2
75 CRA/ROS k_b .	EX	298	(3.1±0.4)(8)			2
75 CRA/ROS k_c .	EX	298	(4.2±0.5)(8)			2
75 CRA/ROS k_d . Upper-limit k.	EX	298	≤4.0(-2)			2
75 CRA/ROS k_e .	EX	298	(3.3±0.6)(8)			2
75 CRA/ROS $k_a + k_b + k_c + k_d + k_e$.	EX	298	(1.52±0.07)(9)			2
Vibrationally excited Vinylcyclopropane formed by:						
$^1\text{CH}_2 + \text{CH}_2=\text{CHCH}=\text{CH}_2$.						
 $\rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2=\text{C}=\text{CH}_2$ (a) \rightarrow  (b)						
Spiropentane \rightarrow Ethene + 1,2-Propadiene (a) \rightarrow Cyclobutane, methylene- (b)						
72 FLO/GIB ¹⁾ k_a . P = 0.9 torr. Decomposition.	EX	664	2.41(-4)			1
72 FLO/GIB ¹⁾ k_a . P = 335 torr. Decomposition.	EX	664	4.58(-5)			1
72 FLO/GIB ¹⁾ k_a . Decomposition. RRKM Calculation.	CO	643-703	7.94(13)	0	27932	1
72 FLO/GIB ¹⁾ k_b . P = 0.9 torr. Isomerisation.	EX	664	3.98(-4)			1
72 FLO/GIB ¹⁾ k_b . P = 335 torr. Isomerisation.	EX	664	7.01(-4)			1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

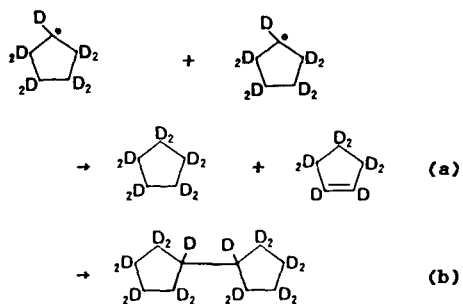
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
<p>1) Pyrolysis in a static system. Gas-chromatography. Other k's, at various pressures in the (0.9-335) torr. range, with or without added CF₂ClCF₂Cl, added as inert gas, are tabulated for both, channel (a) and (b).</p>						
<p>[CH₂CH=CHCH₂CH₃ = CH₂=CHCHCH₂CH₃] → CH₂=CHCH=CH₂ + CH₃</p>						
<p>[2-Pentenyl = 2-Propenyl, 1-ethyl]</p>						
81 BAL/WAL1 Oxidation of 1-Pentene in H ₂ /O ₂ mixtures in aged boric-acid-coated vessels.	ES	753	3.6(3)			1
<p>[CH₂CH=CHCH₂CH₃ = CH₂=CHCHCH₂CH₃] + O₂ → CH₂=CHCH=CHCH₃ + HO₂</p>						
<p>[2-Pentenyl = 2-Propenyl, 1-ethyl-] + Oxygen molecule</p>						
80 BAL/BEN2 Oxidation of 1-Pentene and cis-2-Pentene in aged boric-acid-coated vessels. Gas-chromatography. Gas-chromatography. P(Total) = 500 torr. Same data in 81 BAL/WAL1.	ES	753	2.1(9)			2
<p>CH₂CH=CHCH₂CH₃ + CH₃CHO → CH₃CH₂CH₂CH=CH₂ + CH₃CO (a) → cis-CH₃CH₂CH=CHCH₃ + CH₃CO (b) → trans-CH₃CH₂CH=CHCH₃ + CH₃CO (c)</p>						
<p>2-Pentenyl + Acetaldehyde</p>						
80 RIC/MAR ¹⁾	ES	768	5.01(8)			2
80 RIC/MAR ¹⁾	ES	768	≈1.0(12)	0	6039	2
<p>¹⁾ k_a + k_b + k_c. Acetaldehyde pyrolysis in presence of 1,3-Butadiene, in a static system. The k's estimated by combining the present data with data found in the literature. P(1,3-Butadiene) = 20 torr. P(Acetaldehyde) = 100 torr.</p>						
<p>CH₃CH=CHCH₂CH₂ → CH₃CH₂CH=CHCH₂ (a) → CH₃CH₂CHCH=CH₂ (b)</p>						
<p>3-Pentenyl</p>						
75 STE/RAB k _a + k _b .	ES	298	2.0(9)			1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger \rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_2\text{CH}=\text{CH}_2$ (a)						
 (b)						
4-Pentenyl \rightarrow Ethene + 2-Propenyl (Allyl) (a)						
\rightarrow Cyclopentyl (b)						
72 WAT/OLS ¹⁾ k_a . Decomposition.	EX	319	2.2(9)			1
72 WAT/OLS ¹⁾ k_b . Cyclization. (Intramolecular addition.)	EX	319	2.4(8)			1
¹⁾ Azo-n-propane Photolysis. $\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger$ formed from $\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}^\dagger$ by isomerization, with an average excess vibrational energy of 46 kcal.mol ⁻¹ . In its turn, $\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}^\dagger$ formed by $\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}=\text{CH}$. P = (90-480) torr.						
$\text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2^\dagger \rightarrow \text{CH}_3 + \text{CH}_2=\text{CHCH}=\text{CH}_2$						
3-Butenyl, 1-methyl-						
74 CAR/TAR $\text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2^\dagger$ formed by H + $\text{CH}_2\text{CHCH}_2\text{CH}=\text{CH}_2$.	ES	298	(3.60±0.36)(6)			1
$\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2^\dagger \rightarrow \text{CH}_3 + \text{CH}_2=\text{CHCH}=\text{CH}_2$						
3-Butenyl, 2-methyl-						
74 CAR/TAR $\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}=\text{CH}_2^\dagger$ formed by isomerization from $\text{CH}_3\text{CHCH}_2\text{CH}=\text{CH}_2^\dagger$, in its turn formed by H + $\text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$.	ES	298	(3.60±0.36)(6)			1
 + 						
\rightarrow  +  (a)						
\rightarrow  (b)						
Cyclopentyl + Cyclopentyl						
\rightarrow Cyclopentane + Cyclopentene (a)						
\rightarrow 1,1'-Bicyclopentyl (b)						
82 FUJ/GAE k_a/k_b . H_2O /Cyclopentane gas-phase radiolysis, in a cylindrical Pyrex vessel. Gas-chromatography.	RL	398-443	7.3(-1)	0	<500	2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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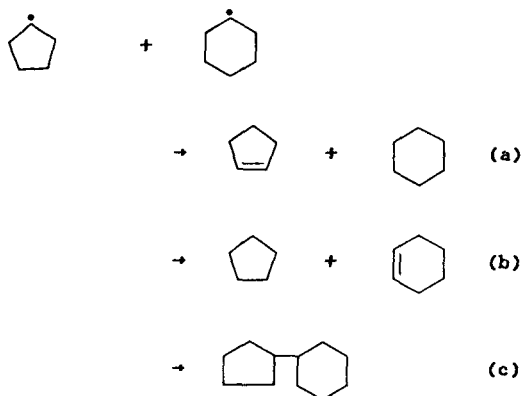
Cyclopentyl-d₉ + Cyclopentyl-d₉
 → Cyclopentane-d₁₀ + Cyclopentene-d₈ (a)
 → 1,1'-Bicyclopentyl-d₁₈ (b)

82 FUJ/GAE RL 398-443 5.8(-1) 0 <500 2/2

k_a/k_b .

H₂O/Cyclopentane-d₁₀ gas-phase pyrolysis,
 in a cylindrical Pyrex vessel.

Gas-chromatography.



Cyclopentyl + Cyclohexyl
 → Cyclopentene + Cyclohexane (a)
 → Cyclopentane + Cyclohexene (b)
 → Cyclohexane, cyclopentyl- (c)

82 FUJ/GAE ¹⁾ RL 398-443 3.3(-1) 0 <500 2/2

k_a/k_c .

82 FUJ/GAE ¹⁾ RL 398-443 2.8(-1) 0 <500 2/2

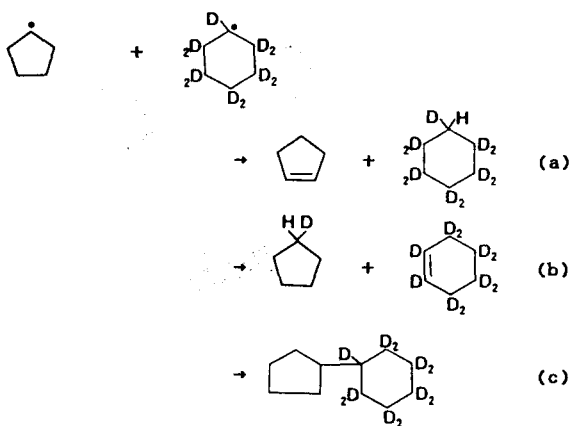
k_b/k_c .

¹⁾ H₂O/Cyclopentane/Cyclohexane gas-phase
 pyrolysis, in a cylindrical Pyrex vessel.

Gas-chromatography.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A k err. units factor
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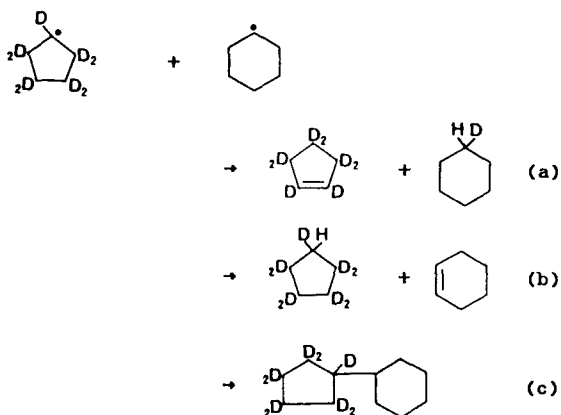
Cyclopentyl + Cyclohexyl-d₁₁

- \rightarrow Cyclopentene + Cyclohexane-d₁₁ (a)
- \rightarrow Cyclopentane-d + Cyclohexene-d₁₀ (b)
- \rightarrow Cyclohexane-d₁₁, cyclopentyl- (c)

82 FUJ/GAE ¹⁾ k_a/k_c . RL 398-443 3.5(-1) 0 <500 2/2

82 FUJ/GAE ¹⁾ k_b/k_c . RL 398-443 2.4(-1) 0 <500 2/2

¹⁾ H₂O/Cyclopentane/Cyclohexane-d₁₂ gas-phase radiolysis, in a cylindrical Pyrex vessel. Gas-chromatography.



Cyclopentyl-d₉ + Cyclohexyl

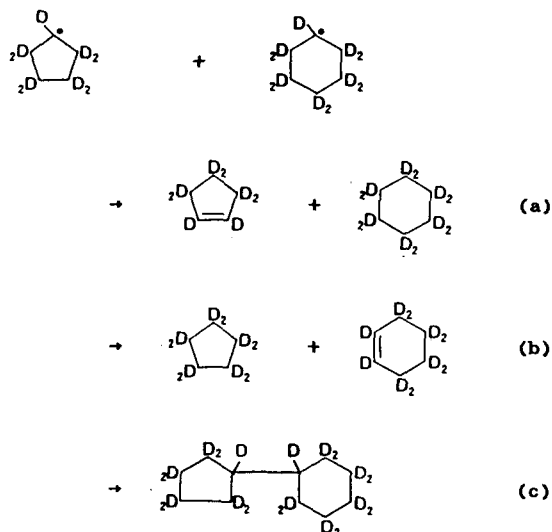
- \rightarrow Cyclopentene-d₉ + Cyclohexane-d (a)
- \rightarrow Cyclopentane-d₉ + Cyclohexene (b)
- \rightarrow Cyclohexane, cyclopentyl-d₉- (c)

82 FUJ/GAE ¹⁾ k_a/k_c . RL 398-443 2.5(-1) 0 <500 2/2

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 FUJ/GAE ¹⁾ k _b /k _c .	RE	398-443	2.8(-1)	0	<500	2/2

¹⁾ H₂O/Cyclopentane-d₁₀/Cyclohexane
gas-phase radiolysis, in a cylindrical
Pyrex vessel.
Gas-chromatography.

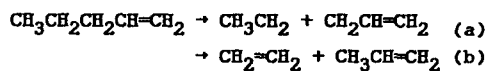


Cyclopentyl-d₉ + Cyclohexyl-d₁₁
→ Cyclopentene-d₈ + Cyclohexane-d₁₂ (a)
→ Cyclopentane-d₁₀ + Cyclohexene-d₁₀ (b)
→ Cyclohexane-d₁₁, cyclopentyl-d-g- (c)

82 FUJ/GAE ¹⁾ k _a /k _c .	RL	398-443	2.8(-1)	0	<500	2/2
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82 FUJ/GAE ¹⁾ k _b /k _c .	RL	398-443	2.4(-1)	0	<500	2/2
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¹⁾ H₂O/Cyclopentane-d₁₀/Cyclohexane-d₁₂
gas-phase radiolysis, in a cylindrical
Pyrex vessel.
Gas-chromatography.

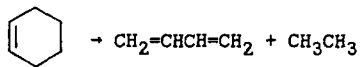


1-Pentene



73 SHI/KIN1 k _a .	ES	753-1023	3.16(15)	0	35732	1
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78 TSA2 ¹⁾ k _a .	EX	1000-1200	(1.0±0.1)(16)	0	35900	1
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4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
78 TSA2 ¹⁾ k _b .	EX	1000-1200	(3.16±0.95)(12)	0	28900	1
¹⁾ 1-Pentene/Cyclohexene/Toluene/Ar thermolysis in a shock-tube. k determined relative to the reaction:						
 $\text{Cyclohexene} \rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{CH}_3$						
P(Ar) ~ (1.7-5) atm. [1-Pentene] = 0.01%. [Cyclohexene] = 0.005%. [Toluene] = 1%.						
73 SHI/KIN1 k _{overall} .	EX	753-1023	1.58(12)	0	26170	1
$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}=\text{CHCH}_2 + \text{CH}_3$ (a) → any other products (b)						
2-Pentene (cis-trans mixture)						
72 SHI/AMA k _a .	ES	753-1003	3.16(15)	0	36236	1
72 SHI/AMA k _{overall} .	EX	753-1003	2.0(12)	0	26673	1
cis-CH ₃ CH ₂ CH=CHCH ₃ (+ M) → trans-CH ₃ CH ₂ CH=CHCH ₃ (+ M)						
2-Pentene, (Z)-						
74 SPR/AKI M = NO ₂ .	EX	298-381	3.12(10)	0	5652±46'	2 1.15
trans-CH ₃ CH ₂ CH=CHCH ₃ (+ M) → cis-CH ₃ CH ₂ CH=CHCH ₃ (+ M)						
2-Pentene, (E)-						
74 SPR/AKI	EX	298-382	5.25(10)	0	6281±44	2 1.15
CH ₃ CH ₂ C(CH ₃)=CH ₂ → CH ₃ + CH ₂ C(CH ₃)=CH ₂						
1-Butene, 2-methyl-						
77 TRE/WRI Limiting high-pressure k.	EX	671-722	3.98(16)	0	35732±403	1 2.51
CH ₃ CH ₂ C(CH ₃)=CH ₂ [†] → CH ₃ + CH ₂ C(CH ₃)=CH ₂						
1-Butene, 2-methyl-						
71 TAY/SIM ¹⁾ A7 366 nm.	EX	298	(5.94±0.59)(7)			1
71 TAY/SIM ¹⁾ At 435.8 nm.	EX	298	(3.42±0.34)(7)			1
¹⁾ CH ₃ CH ₂ C(CH ₃)=CH ₂ [†] formed by ¹ CH ₂ + (CH ₃) ₂ C=CH ₂ . Unreported T assumed to be 287 K.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_2\text{CHCH}=\text{CH}_2 \xrightarrow{\dagger} \text{CH}_3 + \text{CH}_3\text{CHCH}=\text{CH}_2$							
1-Butene, 3-methyl-							
71 TAY/SIM ¹⁾ At 366 nm.	EX	298	(1.74±0.44)(8)			1	
71 TAY/SIM ¹⁾ At 435.8 nm.	EX	298	(1.01±0.25)(8)			1	
¹⁾ (CH ₃) ₂ formed by isomerization from 1,1-dimethylcyclopropane which, in its turn, was formed by ¹ CH ₂ + (CH ₃) ₂ C=CH ₂ . Unreported T assumed to be 298 K.							
			$\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$	(a)			
			$\rightarrow \text{CH}_2=\text{CH}_2 + \triangle$	(b)			
Cyclopentane							
78 TSA2 ¹⁾ k _a . Thermal isomerization.	RN	1000-1200	1.26(16)	0	42700	1	
78 TSA2 ¹⁾ k _a . Thermal isomerization. k unaffected by 1-Pentene decomposition.	CO	1000-1200	6.31(15)	0	42000	1	1.58
78 TSA2 ¹⁾ k _b . Minor channel. Thermolysis.	EX	1000-1200	1.78(16)	0	47840±200	1	1.26
¹⁾ Cyclopentane/Cyclohexene/Ar thermolysis in a single-pulse shock-tube. k determined relative to the reaction:							
			$\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{CH}_3$				
[Cyclohexene] = (0.005-0.01)% [Cyclopentane] = (0.5-2.0)% P(Ar) ~ (1.7-6) atm.							
79 KAL/NAM ²⁾ k _{ref} : CH ₃ CH ₃ → products.	RL	1128-1151	(5.3±1.2)			1/1	
79 KAL/NAM ²⁾ k _{ref} : CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ → products.	RL	1023-1103	(6.7±1.8)(-1)			1/1	
²⁾ k _{overall} /k _{ref} . Cyclopentane/Ethane (or Pentane) pyrolysis in a tubular reactor. Average ratios.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
(a)						
→ cis-CH ₃ CH=CHCH ₂ CH ₃ [†]						
→ trans-CH ₃ CH=CHCH ₂ CH ₃ [†]						
→ CH ₃ CH ₂ C(CH ₃)=CH ₂ [†]						
→ CH ₃ CH=C(CH ₃) ₂ [†]						
Cyclopropane, 1,2-dimethyl-, cis-						
72 GRO/HAS ¹⁾	EX	298	(5.74±0.18)(8)			1
k _a .						
72 GRO/HAS ¹⁾	RL	298	5.03			1/1
k _a /(k _b + k _c + k _d + k _e).						
72 GRO/HAS ¹⁾	EX	298	(1.14±0.11)(8)			1
k _b + k _c + k _d + k _e .						
¹⁾ cis-1,2-Dimethylcyclopropane (Vibrationally excited) formed by ¹ CH ₂ + cis-CH ₂ CH=CHCH ₃ .						
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ → CH ₃ CH ₂ CH ₂ CHCH ₃						
Pentyl						
71 WAT	ES	297-435	3.3(8)	0	7599	1
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ [†] → CH ₃ CH ₂ CH ₂ CHCH ₃ [†]						
Pentyl						
71 WAT ¹⁾	RL	298	8.2			1/1
k _{ref} :						
CH ₃ CH ₂ CH ₂ CHCH ₃ → CH ₃ CH ₂ + CH ₂ =CHCH ₃						
Estimated ratio.						
71 WAT/LAW ¹⁾	EX	330	3.3(6)			1
71 WAT/LAW ¹⁾	EX	373	8.8(6)			1
¹⁾ CH ₃ CH ₂ CH ₂ CH ₂ [†] formed by the Azo-n-propane Photolysis.						
CH ₃ CH ₂ CH ₂ CH ₂ CH ₂ + O ₂ → CH ₃ CH ₂ CH ₂ CH=CH ₂ + HO ₂						
Pentyl + Oxygen molecule						
80 BAL/BEN1	ES	753	2.9(11)			2
Pentane oxidation in aged boric-acid-coated vessels.						
Gas-chromatography.						
P(Total) ~ 500 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2$ → $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a) → $\text{CH}_3(\text{CH}_2)_8\text{CH}_3$ (b)						
Pentyl						
71 WAT ¹⁾	RL	298	1.4(-1)			2/2
71 WAT/LAW ¹⁾	RL	330	1.5(-1)			2/2
¹⁾ k_a/k_b . Azo-n-propane Photolysis.						
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{N}=\text{NCH}_3$ → $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3 + (\cdot\text{C}_5\text{H}_{10})\text{N}=\text{NCH}_3$						
Pentyl + Diazene, methylpentyl-						
71 WAT	ES	297-435	4.2(11)	0	3926	2
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3 \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$						
Butyl, 1-methyl-						
80 BAL/BEN1 Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~500 torr.	ES	753	2.3(5)			1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3^\dagger \rightarrow \text{CH}_3\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$						
Butyl, 1-methyl-						
71 WAT/LAW Azo-n-propane Photolysis. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3^\dagger$ formed by isomerization from $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2^\dagger$, in its turn formed by $\text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_2=\text{CH}_2$.	ES	330	3.0(6)			1
78 WIE/COL ¹⁾ At 7.1 eV.	EX	298	(4.4±0.5)(6)			1
78 WIE/COL ¹⁾ At 7.6 eV.	EX	298	(1.1±0.1)(7)			1
¹⁾ Photolysis in a static system. $\text{CH}_3\text{CH}_2\text{CH}_2\text{CHCH}_3^\dagger$ formed by H + $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$. Gas-chromatography.						
$\text{CD}_3\text{CD}_2\text{CD}_2\text{CD}_3^\dagger \rightarrow \text{CD}_3\text{CD}_2 + \text{CD}_3\text{CD}=\text{CD}_2$						
Butyl-1,2,2,3,3,4,4,4-d ₈ , 1-methyl-d ₃						
78 WIE/COL ¹⁾ At 7.1 eV.	EX	298	(1.2±0.2)(6)			1
78 WIE/COL ¹⁾ At 7.6 eV.	EX	298	(2.9±0.3)(6)			1
¹⁾ Photolysis in a static system. $\text{CD}_3\text{CD}_2\text{CD}_2\text{CD}_3^\dagger$ formed by D + $\text{CD}_3\text{CD}_2\text{CD}_2\text{CD}=\text{CD}_2$. Gas-chromatography.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
CH₃CH₂CH₂CHCH₃ + O₂						
→ CH ₃ CH ₂ CH ₂ CH=CH ₂ + HO ₂ (a)						
→ cis-CH ₃ CH ₂ CH=CHCH ₃ + HO ₂ (b)						
→ trans-CH ₃ CH ₂ CH=CHCH ₃ + HO ₂ (c)						
Butyl, 1-methyl- + Oxygen molecule						
80 BAL/BEN1	RL	753	2.3			2/2
(k _b + k _c)/k _a . Oxidation in aged boric-acid-coated Gas-chromatography. Estimated ratio. P(Total) ~ 500 torr.						
CH₃CH₂CH₂CHCH₃ + CH₃CH₂CH₂CH₂CH₂						
→ CH ₃ (CH ₂) ₂ CH(CH ₃)(CH ₂) ₄ CH ₃ (a)						
→ CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ + CH ₃ CH ₂ CH ₂ CH=CH ₂ (b)						
→ CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ + CH ₃ CH ₂ CH=CHCH ₃ (c)						
Butyl, 1-methyl- + Pentyl						
71 WAT	RL	298	1.41			2/2
(k _a + k _b + k _c)/k _a .						
CH₃CH₂CHCH₂CH₃ → CH₃CH₂CH=CH₂ + CH₃						
Propyl, 1-ethyl-						
80 BAL/BEN1	ES	753	1.57(5)			1
Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.						
CH₃CH₂CHCH₂CH₃ + O₂ → cis-CH₃CH₂CH=CHCH₃ + HO₂ (a)						
→ trans-CH ₃ CH ₂ CH=CHCH ₃ + HO ₂ (b)						
Propyl, 1-ethyl- + Oxygen molecule						
80 BAL/BEN1 ¹⁾	RL	753	(1.55±0.09)(6)			2/1
(k _a + k _b)/k _{ref} . k _{ref} : CH ₃ CH ₂ CHCH ₂ CH ₃ → CH ₃ CH ₂ CH=CH ₂ + CH ₃						
80 BAL/BEN1 ¹⁾	ES	753	2.42(11)			2
¹⁾ Oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.						
(CH₃)₃CCH₂ (+ M) → (CH₃)₂C=CH₂ + CH₃ (+ M)						
Propyl, 2,2-dimethyl-						
75 SZI/MAR1	ES	512-571	2.0(13)	0	14997±1007	1 6.31
77 MUL/BAR	ES	~753	≈1.0(13)	0	15098	1
Pyrolysis in a static reactor.						
79 SZI/MAR	RN	512-571	2.51(13)	0	14915±962	1 6.31
Pyrolysis of Neopentane in presence of Azoisopropane. P(Total) = (15-300) torr.						

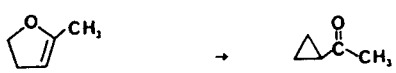
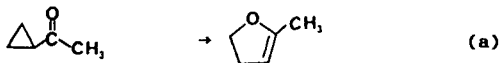

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 FUR/LAI2 ¹⁾ Limiting high-pressure k.	RN	503-608	2.5(13)	0	14595±252	1
72 FUR/LAI2 ¹⁾ Limiting low-pressure k.	RN	503-608	5.8(10)	0	8606±252	2
¹⁾ Hg-photosensitized decomposition of Neopentane. P = (10-280) torr.						
CH₃CH₂CH₂CH₂CH₃ → products						
Pentane						
79 KAL/NAM Pyrolysis of mixtures of Cyclopentane with Ethane and Pentane. k _{ref} : CH ₃ CH ₃ → products.	RL	1103	6.2			1/1
79 ZYC/BAC Pyrolysis in a tubular reactor. P = 1 atm.	EX	1000-1120	6.2(11)	0	26875±201	1
CH₃CH₂CH₂CH₂CH₃[†] → CH₃ + CH₃CH₂CH₂CH₂ (a) → CH₃CH₂ + CH₃CH₂CH₂ (b)						
Pentane						
72 HAS/JOH ¹⁾ k _a + k _b . P = 0.066 torr.	EX	298	(1.5±0.1)(6)			1
72 HAS/JOH ¹⁾ k _a + k _b . P = 0.079 torr.	EX	298	(1.8±0.1)(6)			1
¹⁾ CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ [†] formed by ¹ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₂ CH ₃ .						
(CH₃)₂CHCH₂CH₃[†] → CH₃ + CH₃CH₂CHCH₃ (a) → CH₃ + (CH₃)₂CHCH₂ (b) → CH₃CH₂ + (CH₃)₂CH (c)						
Butane, 2-methyl- (Isopentane)						
72 HAS/JOH ¹⁾ k _a + k _b + k _c . At 366 nm.	EX	298	(3.1±0.2)(6)			1
72 HAS/JOH ¹⁾ k _a + k _b + k _c . At 435.8 nm.	EX	298	(1.6±0.1)(6)			1
¹⁾ (CH ₃) ₂ CHCH ₂ CH ₃ [†] formed by ¹ CH ₂ + (CH ₃) ₃ CH.						
72 HAS/JOH ²⁾ k _a + k _b + k _c . At 366 nm.	EX	298	(2.8±0.1)(6)			1
72 HAS/JOH ²⁾ k _a + k _b + k _c . At 435.8 nm.	EX	298	(2.2±0.1)(6)			1
²⁾ (CH ₃) ₂ CHCH ₂ CH ₃ [†] formed by ¹ CH ₂ + CH ₃ CH ₂ CH ₂ CH ₃ .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_4\text{C} \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3$							
Propane, 2,2-dimethyl- (Neopentane)							
71 BAR/DZI	ES	723-803	6.31(16)	0	41268	1	
73 PAC	EX	793-953	5.01(17)	0	42821±722	1	2.0
76 BRA/WES1	DE	1030-1300	3.3(16)	0	40416	1	1.29
Computer-fit of experimental data.							
76 MAR/PUR	EX	756-845	1.26(16)	0	39694±1804	1	10.0
78 MAR/COM	EX	703-743	3.98(17)	0	42275	1	
Stirred flow-reactor pyrolysis.							
P(Neopentane) = 50 torr.							
78 PAC/WIM	EX	821	(2.4±0.1)(-5)			1	
Neopentane flow-pyrolysis.							
P = 7.6 torr.							
79 BAL/LEW2	EX	1000-1260	2.00(17)	0	40664	1	
VLP-Pyrolysis. Mass spectrometry.							
80 PAC/WIM1	EX	823	(1.7±0.1)(-5)			1	
Pyrolysis of Neopentane in a flow reactor.							
Gas-chromatography.							
P = (4-335) torr.							
81 PRA/ROG	EX	945-1016	1.38(15)	0	40051	1	
Pyrolysis in a wall-less reactor, in Ar.							
P(Ar) = 600 torr.							
$\text{CH}_3\text{C}\equiv\text{CCH}_2\text{COOH} \rightarrow \text{CH}_3\text{CH}=\text{C}=\text{CH}_2 + \text{CO}_2$							
3-Pentynoic acid							
76 BIG/WEA1	EX	500	3.36(-6)			1	
76 BIG/WEA1	EX	662	4.43(-2)			1	
76 BIG/WEA1	EX	500-663	2.47(11)	0	19438±758	1	
A and B recalculated from the reported data.							
$\text{CH}_3\text{C}\equiv\text{CCH}_2\text{COOD} \rightarrow \text{CH}_3\text{CD}=\text{C}=\text{CH}_2 + \text{CO}_2$							
3-Pentynoic acid-d							
76 BIG/WEA1	EX	630	3.30(-3)			1	
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{COOH} \rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CO}_2$							
3,4-Pentadienoic acid							
76 BIG/WEA2	EX	500	3.35(-7)			1	
76 BIG/WEA2	EX	630	1.35(-3)			1	
76 BIG/WEA2	EX	500-715	1.05(11)	0	20152±758	1	2.6
A and B recalculated from the reported data.							

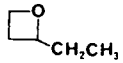

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 Furan, 2,3-dihydro-5-methyl- → Ethanone, 1-cyclopropyl- 73 COC/EGG Pyrolysis. P-independent for P > 4 torr.	EX	672-731	7.07(14)	0	28989±349	1	1.66
 → cis-CH ₃ C(O)CH=CHCH ₃ (b) → trans-CH ₃ C(O)CH=CHCH ₃ (c) → CH ₃ C(O)CH ₂ CH=CH ₂ (d) Ethanone, 1-cyclopropyl- → Furan, 2,3-dihydro-5-methyl- (a) → 3-Penten-2-one, (Z)- (b) → 3-Penten-2-one, (E)- (c) → 4-Penten-2-one (d)							
73 COC/EGG 1)	EX	672-731	7.76(13)	0	27810±349	1	1.7
k _a .							
73 COC/EGG 1)	ES	672-731	6.31(13)	0	28989	1	
k _b .							
73 COC/EGG 1)	ES	672-731	1.58(13)	0	28989	1	
k _c .							
73 COC/EGG 1)	ES	672-731	3.98(14)	0	30071	1	
k _d .							
73 COC/EGG 1)	EX	672-731	2.51(14)	0	29289±505	1	2.14
k _b + k _c + k _d .							
1) Thermal isomerization. P-independent for P > 4 torr.							
 → 2-cyclopenten-1-ol (b) → CH ₂ =CHCHO + CH ₂ =CH ₂ (c) → other products (d) 6-Oxabicyclo[3.1.0]hexane → Cyclopentanone (a) → 2-Cyclopenten-1-ol (b) → 2-Propenal (Acrolein) + Ethene (c) → other products (d)							
74 FLO/PEN1 1)	EX	670-742	1.45(14)	0	28916±180	1	1.29
k _a .							



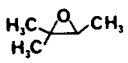
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
74 FLO/PEN1 ¹⁾ k _b .	EX	670-742	3.63(13)	0	29133±265	1	1.45
74 FLO/PEN1 ¹⁾ k _c . The reactant might isomerize to Cyclobutanecarboxaldehyde before decomposing.	EX	670-742	4.07(14)	0	32296±433	1	1.82
74 FLO/PEN1 ¹⁾ k _a + k _b + k _c + k _d .	EX	670-742	2.00(14)	0	28989±108	1	1.17
¹⁾ Thermolysis. P = (1-28) torr.							
CH₃CH=CHCH₂COOH → CH₃CH=CHCH₃ + CO₂ 3-Pentenoic acid							
76 BIG/WEA1	EX	500	2.01(-7)			1	
76 BIG/WEA1	EX	693	1.05(-3)			1	
76 BIG/WEA1	EX	500-720	2.34(11)	0	20814±782	1	
A and B recalculated from the reported data.							
CH₃C(O)C(O)CH₂CH₃ → CH₃CO + CH₃CH₂CO (a) → any other products (b)							
2,3-Pentanedione							
74 SCH/KNO	EX	362-398	≈7.94(16)	0	33971±1459	1	10.0
k _a . Order of magnitude estimate: k _a ~ 0.1k _b .							
74 SCH/KNO	EX	362-398	7.94(17)	0	33971±1459	1	10.0
k _{overall} .							
CH₂=C(CH₃)CH₂COOH → (CH₃)₂C=CH₂ + CO₂ 3-Butenoic acid, 3-methyl- → 1-Propene, 2-methyl- + Carbon dioxide							
77 BIG/WEA ¹⁾	RL	500	2.03(1)			1/1	
k/k _{ref} . k _{ref} : CH ₂ =C(CH ₃)CH ₂ COOH → CH ₂ =C(CH ₃) ₂ + CO ₂							
77 BIG/WEA ¹⁾	EX	500	3.05(-5)			1	
¹⁾ Pyrolysis in a flow-reactor. Gas-chromatography.							
△CH₂COOH → CH₃CH₂CH=CH₂ + CO₂ (a) = (b)							
→ (CH ₃) ₂ C=CH ₂ + CO ₂ (c)							
Cyclopropaneacetic acid							
→ 1-Butene + Carbon dioxide (a) = (b)							
→ 1-Propene, 2-methyl- + Carbon dioxide (c)							
80 BIG/FET ¹⁾	EX	725	1.0(-3)			1	
k _a = k _b .							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 BIG/FET ¹⁾ k _c . Upper-limit k.	EX	725	<4.0(-5)			1	
80 BIG/FET ¹⁾ k _a + k _b + k _c .	EX	725	2.0(-3)			1	
80 BIG/FET ¹⁾ k _a + k _b + k _c . A and B recalculated from the reported data.	EX	750-820	2.18(11)	0	23434±722	1	
¹⁾ Pyrolysis in a flow-reactor. NMR-spectrometry.							
CH₃CH₂OCH₂CH=CH₂ → CH₃CHO + CH₃CH=CH₂ 1-Propene, 3-ethoxy-							
74 EGG/VIT2	EX	560-648	6.92(11)	0	21928±388	1	1.95
CH₃CH₂CH₂OCH=CH₂ → CH₃CH=CH₂ + CH₃CHO Propane, 1-(ethenyloxy)-							
74 BAM	EX	653-708	1.32(11)	0	21399±204	1	1.35
Pyrolysis in a static system. Gas-chromatography.							
 → HCHO + CH ₃ CH ₂ CH=CH ₂ (a)							
→ CH ₃ CH ₂ CHO + CH ₂ CH ₂ (b)							
Oxetane, 2-ethyl- → Formaldehyde + 1-Butene (a)							
→ Propanal + Ethene (b)							
77 CLA/HOL	EX	699-752	2.95(14)	0	29652±437	1	1.91
k _a + k _b . Pyrolysis. P = (0.45-32) torr.							
 → HCHO + (CH ₃) ₂ C=CH ₂ (a)							
→ (CH ₃) ₂ CO + CH ₂ =CH ₂ (b)							
Oxetane, 2,2-dimethyl-							
82 HAM/HOL ¹⁾ k _a .	EX	675-744	3.02(13)	0	26715±349	1	1.78
82 HAM/HOL ¹⁾ k _b .	EX	675-744	3.63(15)	0	32549±528	1	2.19
82 HAM/HOL ¹⁾ k _a + k _b .	EX	675-744	6.03(13)	0	27184±325	1	1.74
¹⁾ Pyrolysis. Vacuum-system. P = (7.2-9.2) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CHO}$ (a) $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{HCHO}$ (b) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{HCHO}$ (c)							
Oxetane, 2,3-dimethyl-, cis-							
\rightarrow 1-Propene + Acetaldehyde (a)							
\rightarrow 2-Butene, (Z)- + Formaldehyde (b)							
\rightarrow 2-Butene, (E)- + Formaldehyde (c)							
74 HOL/SCO ¹⁾	EX	688-756	5.01(15)	0	31815±312	1	1.69
k_a .							
74 HOL/SCO ¹⁾	EX	688-756	1.74(15)	0	31451±360	1	1.78
$k_b + k_c$.							
¹⁾ Pyrolysis. High-vacuum system. $P_0 = (2-32)$ torr.							
 $\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CHO}$ (a) $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{HCHO}$ (b) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3 + \text{HCHO}$ (c)							
Oxetane, 2,3-dimethyl-, trans-							
\rightarrow 1-Propene + Acetaldehyde (a)							
\rightarrow 2-Butene, (Z)- + Formaldehyde (b)							
\rightarrow 2-Butene, (E)- + Formaldehyde (c)							
74 HOL/SCO	EX	688-756	8.13(15)	0	32537±334	1	1.78
k_a .							
74 HOL/SCO	EX	688-756	3.09(15)	0	32046±375	1	1.82
$k_b + k_c$.							
¹⁾ Pyrolysis. High-vacuum system. $P_0 = (2-32)$ torr.							
 $\rightarrow (\text{CH}_3)_3\text{CCHO}$ (a) $\rightarrow (\text{CH}_3)_2\text{CHC(O)CH}_3$ (b) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{OCH}_2\text{CH}_3$ (c) $\rightarrow (\text{CH}_3)_2\text{C(OH)CH}=\text{CH}_2$ (d) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH(OH)CH}_3$ (e)							
Oxirane, trimethyl-							
\rightarrow Propanal, 2,2-dimethyl- (a)							
\rightarrow 2-Butanone, 3-methyl- (b)							
\rightarrow 1-Propene, 2-ethoxy- (c)							
\rightarrow 3-Buten-2-ol, 2-methyl- (d)							
\rightarrow 3-Buten-2-ol, 3-methyl- (e)							
75 FLO/OEZ ¹⁾	EX	665-715	1.07(13)	0	27208±421	1	1.82
k_a .							
75 FLO/OEZ ¹⁾	EX	665-715	1.12(13)	0	27052±601	1	2.40
k_b .							

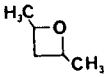
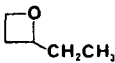

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
75 FLO/OEZ ¹⁾ k _c .	EX	665-715	1.51(13)	0	27738±457	1	1.95
75 FLO/OEZ ¹⁾ k _d .	EX	665-715	1.02(12)	0	27533±373	1	1.70
75 FLO/OEZ ¹⁾ k _e .	EX	665-715	8.71(11)	0	25681±986	1	4.17
75 FLO/OEZ ¹⁾ k _a + k _b + k _c + k _d + k _e .	EX	665-715	6.31(13)	0	27473±505	1	2.09
¹⁾ Thermolysis. Static system. P = (1.5-27) torr.							
CH₃OCH₂CH₂OCH=CH₂ → CH₃OCH=CH₂ + CH₃CHO							
Ethene, (2-methoxyethoxy)-							
74 BAM Pyrolysis in a static system. Gas-chromatography.	EX	653-708	1.38(11)	0	22241±144	1	1.23
CH₃C(O)OCH₂CH₂CH₃ → CH₃COOH + CH₃CH=CH₂							
Acetic acid propyl ester (n-Propyl acetate)							
76 DEB/TAY	EX	650-700	4.47(12)	0	24409	1	
CH₃C(O)OCH(CH₃)₂ → CH₃COOH + CH₃CH=CH₂							
Acetic acid 1-methylethyl ester (i-Propyl acetate)							
75 TAY Pyrolysis. CH ₃ COOH decomposes fast to CO ₂ + CH ₄ .	EX	609-657	1.58(13)	0	23020±302	1	1.58
77 SMI/MUT	EX	651	(5.93±0.17)(-3)			1	
78 TAY Pyrolysis in a stainless-steel reactor.	EX	609-668	1.62(13)	0	22994	1	
82 MCM/LEW Ethyl acetate/Isopropyl acetate/Isobutyl bromide/SF ₆ /CO ₂ laser-powered homogeneous pyrolysis. P(Acetate, or Bromide) ~1.0 torr. P(SF ₆) = 4 torr. P(CO ₂) = 93 torr.	EX	950-1000	5.01(12)	0	22496	1	
CH₃CH₂C(O)OH₂CH₃ → CH₃CH₂COOH + CH₂=CH₂							
Propanoic acid ethyl ester							
76 BAR/COC Reflected shock-waves in single-pulse shock-tubes. Curved Arrhenius plot above 1100 K.	EX	919-1220	5.25(12)	0	24418	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH₃CH₂OC(O)OCH₂CH₃ → CH₂=CH₂ + CO₂ + CH₃CH₂OH							
Carbonic acid diethyl ester (Diethyl carbonate)							
72 BIG/WRE1 ¹⁾ Sealed-tube pyrolysis.	EX	554-594	1.43(13)	0	23352	1	
72 BIG/WRE1 ¹⁾ Flow-tube pyrolysis.	EX	700	(7.40±0.22)(-2)			1	
72 BIG/WRE1 ¹⁾ Flow-tube pyrolysis. The A-factor recalculated from reported data.	EX	663-708	(4.05±0.12)(13)	0	23754	1	
¹⁾ Diethyl carbonate pyrolysis.							
76 CRO/HUN	EX	584-663	1.15(13)	0	23456	1	
CH₃C(O)OCH₂CH₂OCH₃ → CH₃COOH + CH₂=CHOCH₃							
Ethanol, 2-(methoxy)-, acetate							
76 DEB/TAY	EX	650-700	7.94(12)	0	25767	1	
80 CHU/MAR Gas phase pyrolysis in a static system. Gas-chromatography. P = (63-207) torr.	EX	592-723	1.09(12)	0	24502±352	1	1.74
HOCH₂C(O)OCH(CH₃)₂ → HOCH₂COOH + CH₃CH=CH₂							
Acetic acid, hydroxy-, 1-methylethyl ester							
77 CHU/MAR	EX	563-623	3.63(12)	0	21641±352	1	1.91
CH₃CH₂C(CH₃)₂O → CH₃CH₂ + (CH₃)₂CO (a) → CH₃CH₂COCH₃ + CH₃ (b)							
Propoxy, 1,1-dimethyl-							
78 BAT/ISL1 ¹⁾ k _a .	EX	433-463	5.01(14)	0	7197±503	1	1.58
78 BAT/ISL1 ¹⁾ k _a /k _b .	RL	433	(8.0±0.5)(1)			1/1	
79 BAT ¹⁾ k _a .	EX	393-433	6.31(14)	0	6945±500	1	3.16
78 BAT/ISL1 ¹⁾ k _b .	RN	433	1.0(15)	0	9411	1	
¹⁾ Pyrolysis in a static system. Gas-chromatography.							
CH₃CH₂C(CH₃)₂O + NO → CH₃CH₂C(CH₃)₂ONO							
Propoxy, 1,1-dimethyl- + Nitrogen oxide (NO)							
78 BAT/ISL1 Pyrolysis in a static system. Gas-chromatography. Calculated from k ₁ = k ₋₁ K.	DE	393-428	3.16(13)	0	0	2	1.58

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{CCH}_2\text{OO} \rightarrow (\text{CH}_3)_2\text{C}(\text{CH}_2\text{OOH})\text{CH}_2$ (a) $\rightarrow (\text{CH}_3)_2\text{CCH}_2(\text{O})\text{OCH}_3$ (b)						
Propyldioxy, 2,2-dimethyl-						
75 BAK/BAL1 k_a .	ES	753	1.85(4)			1
75 BAK/BAL1 k_a .	ES	298-753	1.26(12)	0	13588	1
75 BAK/BAL1 k_b . Upper-limit k.	ES	753	$\leq 1.6(3)$			1
$\text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{CHCH}_3 \rightarrow$  + OH						
Butyl, 3-hydroperoxy-1-methyl- \rightarrow Oxetane, 2,4-dimethyl- + Hydroxyl						
80 BAL/BEN1 Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.	ES	753	1.0(6)			1
$\text{HOOCCH}_2\text{CH}_2\text{CHCH}_2\text{CH}_3 \rightarrow$  + OH						
Propyl, 3-hydroperoxy-1-ethyl, \rightarrow Oxetane, 2-ethyl- + Hydroxyl						
80 BAL/BEN1 Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.	ES	753	1.0(6)			1
$(\text{CH}_3)_2\text{C}(\text{CH}_2\text{OOH})\text{CH}_2 \rightarrow$  + OH						
Propyl, 2-methyl-2-hydroperoxymethyl- \rightarrow Oxetane, 3,3-dimethyl-						
75 BAK/BAL1	ES	753	1.0(6)			1 2.0
75 BAK/BAL1	ES	298-753	6.31(11)	0	10065	1 2.0
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OO} \rightarrow \text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OOH}$ (a) $\rightarrow \text{CH}_3\text{CHCH}_2\text{CH}_2\text{CH}_2\text{OOH}$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{CHCH}_2\text{CH}_2\text{OOH}$ (c)						
Pentyldioxy						
80 BAL/BEN1 ¹⁾ k_a/k_c .	RL	753	$(3.1 \pm 0.4)(-1)$			1/1


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
80 BAL/BEN1 ¹⁾ k _a .	RN	753	9.3(4)			1	
80 BAL/BEN1 ¹⁾ k _b /k _c .	RL	753	(2.2±0.3)			1/1	
80 BAL/BEN1 ¹⁾ k _b .	RN	753	6.6(5)			1	
80 BAL/BEN1 ¹⁾ k _c .	ES	753	3.0(5)			1	
CH₃CH₂CH₂CH(OO·)CH₃ → CH₃CH₂CHCH(OOH)CH₃ (a) → CH₃CHCH₂CH(OOH)CH₃ (b)							
Butyldioxy, 1-methyl-							
80 BAL/BEN1 ¹⁾ k _a /k _b .	RL	753	(6.3±2.5)			1/1	
80 BAL/BEN1 ¹⁾ k _a .	RN	753	4.7(5)			1	
80 BAL/BEN1 ¹⁾ k _b .	ES	753	3.0(5)			1	
¹⁾ Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.							
CH₃CH(OOH)CH₂CH(OO·)CH₃ → CH₃CHO + CH₃CHO + HCHO + OH							
Butyldioxy, 3-hydroperoxy-1-methyl-							
80 BAL/BEN1	ES	753	5.0(5)			1	
Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) ~ 500 torr.							
CH₃CH₂CH(OO·)CH₂CH₂OOH → CH₃CH₂CHO + HCHO + HCHO + OH							
Propyldioxy, 3-hydroperoxy-1-ethyl-							
80 BAL/BEN1	ES	753	8.0(5)			1	
Pentane oxidation in aged boric-acid-coated vessels. Gas-chromatography. P(Total) = ~ 500 torr.							
(CH₃)₂C(CH₂OOH)CH₂OO → (CH₃)₂CO + 2HCHO + OH							
Propyldioxy, 2-hydroperoxymethyl-2-methyl-							
75 BAK/BAL1	ES	753	1.5(6)			1	2.0
75 BAK/BAL1	ES	298-753	6.31(11)	0	9562	1	2.0
(CH₃)₃COCH₃ → (CH₃)₂C=CH₂ + CH₃OH							
Propane, 2-methoxy-2-methyl-							
74 CHO/GOL	EX	780-917	7.94(13)	0	29693±503	1	
The A and B factors are recommended for T = 800 K.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

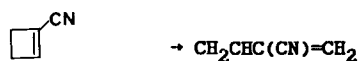
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$\text{CH}_3\text{COSCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$ Ethanethioic acid S-(1-methylethyl) ester	72 OEL/TIN	EX 723-799	1.58(13)	0	24761	1	
Elimination by thermolysis.							
$\text{CH}_3\text{C}(\text{S})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{COSCH}(\text{CH}_3)_2$ (b)	75 BIG/GAB ¹⁾	EX 629	5.12(-1)			1	
k_a . Elimination.							
75 BIG/GAB ¹⁾	EX 563-583	7.94(12)		0	19099	1	
k_a . Elimination.							
75 BIG/GAB ¹⁾	EX 559	1.01(-2)				1	
$k_a + k_b$. Overall reaction.							
75 BIG/GAB ¹⁾	EX 563-583	7.08(12)		0	19099	1	
$k_a + k_b$. Overall reaction.							
¹⁾ Flow reactor pyrolysis.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{SCH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHSCH}_3$ Ethanol, 2-(methylthio)-, acetate	80 CHU/MAR	EX 592-723	1.86(11)	0	21531±553	1	2.45
Pyrolysis. Static system. P = (63-207) torr.							
$\text{CH}_3\text{C}(\text{O})\text{SCH}(\text{CH}_3)\text{OCH}_3 \rightarrow \text{CH}_3\text{C}(\text{S})\text{OH} + \text{CH}_2=\text{CHOCH}_3$ (a) $\rightarrow \text{CH}_3\text{COSH} + \text{CH}_2=\text{CHOCH}_3$ (b)	72 OEL/TIN	EX 583-633	1.00(13)	0	19930	1	
$k_a + k_b$. Thermolysis.							
$\text{CH}_3\text{OC}(\text{S})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OH} + \text{COS} + \text{CH}_3\text{CH}=\text{CH}_2$ Carbonothioic acid O-methyl O-(1-methylethyl) ester	82 ALA/BIG ¹⁾	EX 629	1.5			1	
82 ALA/BIG ¹⁾	EX 500-560	1.19(11)		0	15785	1	
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a flow reactor. IR-spectrometry. P = (2-800) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
CH₃OC(O)SCH(CH₃)₂ → CH₃OH + COS + CH₃CH=CH₂							
Carbonothioic acid O-methyl S-(1-methylethyl) ester							
79 ALA/BIG ¹⁾	EX	629	4.6(-5)				1
79 ALA/BIG ¹⁾	EX	713-753	9.04(12)	0	25047±722		1
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a flow-reactor.							
IR-spectrometry.							
(CH₃)₂CHOC(O)SCH₃ → CH₃CH=CH₂ + CO₂ + CH₃SH							
Carbonothioic acid S-methyl O-(1-methylethyl) ester							
79 ALA/BIG ¹⁾	EX	629	9.4(-3)				1
79 ALA/BIG ¹⁾	EX	820-857	7.27(11)	0	20115±1203		1
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a Flow-reactor.							
IR-spectrometry.							
							
→ CH₃CH=CH₂ + CH₂=CH₂ + SO₂							
Thiophene, tetrahydro-3-methyl-1,1-dioxide-							
(3-Methylsulfolane)							
→ 1-Propene + Ethene + Sulfur dioxide							
75 COR/TSA	EX	733-798	1.3(16)	0	33200±750	1	2.51
Pyrolysis in a flow-tube reactor.							
CH₃SC(S)OCH(CH₃)₂ → CH₃SH + COS + CH₃CH=CH₂							
Carbonodithioic acid S-methyl O-(1-methylethyl) ester							
82 ALA/BIG ¹⁾	EX	629	5.6(-1)				1
82 ALA/BIG ¹⁾	EX	500-550	1.39(12)	0	17950		1
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a flow reactor.							
IR-spectrometry.							
P = (2-800) torr.							
CH₃OC(S)SCH(CH₃)₂ → CH₃OH + CS₂ + CH₃CH=CH₂							
Carbonodithioic acid O-methyl S-(1-methylethyl) ester							
82 ALA/BIG ¹⁾	EX	629	7.9(-1)				1
82 ALA/BIG ¹⁾	EX	580-630	7.40(11)	0	20235		1
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a flow reactor.							
IR-spectrometry.							
P = (2-800) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

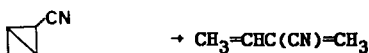
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
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1-Cyclobutene-1-carbonitrile

→ 3-Butenenitrile, 2-methylene-

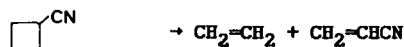
72 SAR/GAL ¹⁾	EX	463-498	2.51(13)	0	16910	1
72 SAR/GAL ¹⁾	SE	463-498	2.39(13)	0	16910	1

Average value of previous
and present data.¹⁾ Thermal isomerization in a flow-reactor.
Gas-chromatography.

Bicyclo[1.1.0]butane-1-carbonitrile

→ 3-Butenenitrile, 2-methylene-

72 SAR/GAL ¹⁾	EX	726-783	7.94(13)	0	20181	1
72 SAR/GAL ¹⁾	SE	726-783	8.43(13)	0	20181	1

Average value of previous
and present data.¹⁾ Thermal isomerization in a flow-reactor.
Gas-chromatography.

Cyclobutanecarbonitrile → Ethene + 2-Propenenitrile



72 SAR/GAL ¹⁾	EX	726-783	2.03(15)	0	28535	1
72 SAR/GAL ¹⁾	SE	726-783	3.16(15)	0	28535	1

Average value of previous
and present data.¹⁾ Thermal isomerization in a flow-reactor.
Gas-chromatography.




75 KIN/GOD3 ²⁾	EX	833-1203	1.0(15)	0	28686±503	1
75 KIN/GOD3 ²⁾	EX	833-1203	7.94(15)	0	29743±503	1

Based on the present VLPP results
and previous high-pressure data.Based on combination of present
and previous VLPP data.²⁾ VLP-Pyrolysis system.
P = (0.1-1.0) mtorr.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

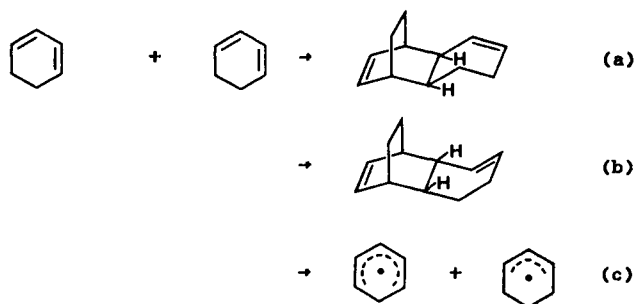
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CCH}_2\text{CN} \rightarrow (\text{CH}_3)_2\text{CH} + \text{CH}_2\text{CN}$ Butanenitrile, 3-methyl- 75 KIN/GOD2	EX	1011-1123	2.51(15)	0	36789±856	1 2.0
$(\text{CH}_3)_3\text{CCN} \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{HCN}$ (a) $\rightarrow (\text{CH}_3)_2\text{CCN} + \text{CH}_3$ (b) Propanenitrile, 2,2-dimethyl- 73 DAS/EMO k_a 76 KIN/GOD k_a 76 KIN/GOD k_b	EX	838-927	1.58(12)	0	32053±247	1 1.02
	EX	1023-1254	1.26(14)	0	37292±805	1 2.0
	EX	1023-1254	7.94(15)	0	37695±805	1 2.0
$\text{CH}_3\text{CH}_2\text{N}=\text{NCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{CH} + \text{N}_2$ Diazene, ethyl-(1-methylethyl)- 77 MAR/MAC Thermolysis in a vacuum system.	EX	533-593	3.16(16)	0	24779±361	1 3.16
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{NH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2 + \text{NH}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2 + (\text{CH}_3)_2\text{CNH}_2$ (b) $\rightarrow (\text{CH}_3)_2\text{C}=\text{CHCH}_3 + \text{NH}_3$ (c) 2-Butanamine, 2-methyl- (t-Amylamine) 78 TSA1 1) k_a 78 TSA1 1) k_b 78 TSA1 1) k_c . Upper-limit k.	EX	990-1200	7.94(15)	0	39700±500	1 2.0
	EX	990-1200	3.16(16)	0	38500±500	1 2.0
	EX	990-1200	<3.16(14)	0	37200	1
1) t-Amylamine/4-Methylcyclohexene (or Hexene)/ Toluene/Ar thermolysis in a shock-tube. k's deterative to either of the two reactions:						
						
$\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$						
						
$\rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_2=\text{CH}_2$						
[t-Amylamine] = (0.1-0.4)%. [Cyclohexene = 1%, or [4-Methylcyclohexene] = 0.025%. [Toluene + Argon] = 1%.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CN} \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CNCN}$ Propanenitrile, 3-(acetyloxy)- 80 CHU/MAR Gas phase pyrolysis in a static system. Gas-chromatography. P = (63-207) torr.	EX	592-723	3.24(11)	0	20677±204	1	1.35
$\text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)_2\text{ONO} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)\text{O} + \text{NO}$ Nitrous acid 1,1-dimethylpropyl ester (1,1-dimethyl- propyl nitrite) 78 BAT/ISL1 Pyrolysis in a static system. Gas-liquid chromatography.	EX	393-428	2.00(16)	0	20280±50	1	1.26
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OCH}_2\text{CH}_3 \rightarrow (\text{CH}_3)_2\text{NH} + \text{CO}_2 + \text{CH}_2=\text{CH}_2$ Carbamic acid, dimethyl-, ethyl ester 72 DAL/ZIO2 Thermolysis in a conventional static system.	EX	323-333	1.26(12)	0	22315±201	1	
$\text{trans-CH}_2=\text{CHCH}=\text{CHCH}=\text{CH}_2 \rightarrow$ 							
1,3,5-Hexatriene, (E)- → 1-3-Cyclohexadiene 73 DOE/BEA Thermal isomerization in a 12 liter Pyrex flask, or in a 3.5 liter corning lead-potash flask. Gas-chromatography.	EX	533-573	8.13(12)	0	22295±604	1	2.95
81 GRI/SCH Thermal isomerization in an air thermostat. P = (2-3) torr.	EX	555-606	(2.77±0.53)(13)	0	22914±111	1	
$\text{cis-CH}_3\text{CH}=\text{C}=\text{C}=\text{CHCH}_3 \rightarrow \text{trans-CH}_3\text{CH}=\text{C}=\text{C}=\text{CHCH}_3$ 2,3,4-Hexatriene, (Z)- 76 ROT/EXN	EX	373-423	1.1(13)	0	16004±151	1	
 \rightarrow  $+ \text{H}_2$							
1,3-Cyclohexadiene → Benzene + Hydrogen molecule 73 ALF/BEN VLPP in a triple-aperture quartz reactor. [1,3-Cyclohexadiene] = (0.01-2.0)x10 ¹⁶ molec.cm ⁻³ .	EX	943-1073	2.51(13)	0	29693±503	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
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1,3-Cyclohexadiene + 1,3-Cyclohexadiene

→ exo-Tricyclo[6.2.2.0^{2,7}]dodeca-3,9-diene (a)

→ endo-Tricyclo[6.2.2.0^{2,7}]dodeca-3,9-diene (b)

→ Cyclohexadienyl + 2-Cyclohexen-1-yl (c)

71 DEM/HUY ¹⁾ EX 471-639 1.82(6) 0 12280±136 2 1.29

$k_a + k_b$.

71 DEM/HUY ¹⁾ RL 471-639 1.29 0 -428±91 2/2 1.17

k_b/k_a .

71 DEM/HUY ¹⁾ RN 471-639 9.33(8) 0 12632±252 2 1.78

k_a .

71 DEM/HUY ¹⁾ RN 471-639 1.20(9) 0 12229±252 2 1.78

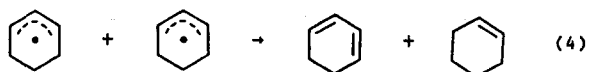
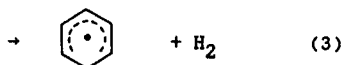
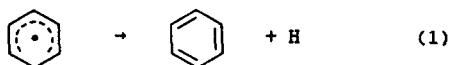
k_b .

¹⁾ Thermal dimerization in Pyrex reaction vessel.

P = (25-630) torr.

72 DEM/HUY ²⁾ ES 512-673 2.51(13) 0 17866±503 2 2.51

k_c . Secondary reactions for channel (c) are:



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data	T/K	k, k/k(ref),	n	B,	k, A k err.
	type		A, A/A(ref)		B-B(ref)	units factor

Cyclohexadienyl

→ Benzene + Hydrogen atom (1)

1,3-Cyclohexadiene + Hydrogen atom

→ 2-Cyclohexen-1-yl (2)

→ Cyclohexadienyl + Hydrogen molecule (3)

2-Cyclohexen-1-yl + 2-Cyclohexen-1-yl

→ 1,3-Cyclohexadiene + Cyclohexene (4)

→ Bi-2-cyclohexen-1-yl (5)

→ Cyclohexene, 3-(4-cyclohexen-1-yl) (6)

Reported rate constant ratios for the 512-673 K T-range (all in $\text{cm}^3\text{mol}^{-1}\text{s}^{-1}$ units) are:

$$k_c k_3 / k_2 = 2.04 \times 10^{12} \exp(-17866 \pm 503) / T \quad (F = 2.51)$$

$$k_c (1 + k_3 / k_2)$$

$$= 1.35 \times 10^{13} \exp(-17866 \pm 50) / T \quad (F = 1.10)$$

based on $[\text{C}_6\text{H}_6]$, or

$$= 1.35 \times 10^{13} \exp(17866 \pm 503) / T \quad (F = 2.51)$$

by computation.

$$k_c k_4 / (k_4 + k_5 + k_6)$$

$$= 1.78 \times 10^{13} \exp(18319 \pm 554) / T \quad (F = 2.51)$$

based on [Cyclohexene], or

$$= 8.32 \times 10^{12} \exp(17866 \pm 503) / T \quad (F = 2.51)$$

by computation.

$$k_c (k_5 + k_6) / (k_4 + k_5 + k_6)$$

$$= 3.31 \times 10^{12} \exp(17916 \pm 906) / T \quad (F = 4.68)$$

based on $[\text{C}_{12}\text{H}_{18}]$, or

$$= 3.02 \times 10^{12} \exp(17866 \pm 50) / T \quad (F = 2.51)$$

by computation.

$\text{C}_{12}\text{H}_{18}$ is probably Bi-2-cyclohexen-1-yl,

or 3-(4-Cyclohexen-1-yl)-cyclohexene.

2) Pyrolysis in a cylindrical Pyrex reaction

vessel. Gas-chromatography.

Mass-spectrometry.

P = (10-500) torr.

All the estimated and computed rate constant

ratios are based on steady-state treatment.

The Cyclohexadienyl radical,



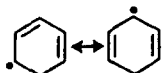
formed in the channel (c) by abstraction of a

H atom from a Methylene group of 1,3-Cyclo-

hexadiene, is resonant between two forms:

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

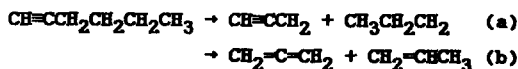
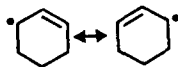
Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
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1,4-, and 1,5-Cyclohexadien-1-yl respectively.
The 2-Cyclohexen-1-yl radical,



also formed in the channel (c) by addition of a H atom to Methylidyne group adjacent to a Methylene group of 1,3-Cyclohexadiene, is resonant with its own mirror image:



1-Hexyne

78 TSA3 ¹⁾ EX 990-1200 7.94(15) 0 36300±500 1 1.58
k_a. Bond-breaking reaction.

78 TSA3 ¹⁾ EX 990-1200 5.01(12) 0 28400±1000 1 2.51
k_b. Molecular reaction.

¹⁾ 1-Hexyne/5-Methyl-1-hexyne/Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to 5-Methyl-1-hexyne decomposition. [1-Hexyne] = 0.04%. [5-Methyl-1-hexyne] = 0.02%. P(Ar) ~ (2-6) atm. [Toluene] = 1%.

81 KIN2 ²⁾ EX 903-1153 7.94(15) 0 35581±1007 1 2.0
k_a. Bond-breaking reaction.

81 KIN2 ²⁾ EX 903-1153 5.01(12) 0 28385±503 1 2.51
k_b. Molecular reaction.

²⁾ 1-Hexyne thermolysis in A VLPP system.



2-Pentyne, 4-methyl-


81 KIN/NGU EX 903-1246 1.58(16) 0 37443±755 1 2.0
4-Methyl-2-pentyne thermolysis in a VLPP system.



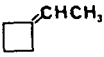


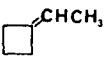
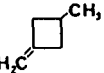
1-Butyne, 3,3-dimethyl-

77 KIN EX 933-1182 6.31(15) 0 35632±755 1 2.0


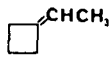
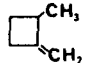
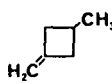
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CH}_2\text{CH}=\text{CHCH}=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_2\text{CH}=\text{CHCH}=\text{CH}_2$ 1,3-Hexadiene						
80 TRE 1,3-Hexadiene pyrolysis in a static system. Gas-chromatography. P = (25-200) torr.	EX	694-759	8.32(15)	0	33412±423	1 1.48
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}_2 + \text{CH}_2=\text{CHCH}_2$ (a) → any other products (b) 1,5-Hexadiene → 2-Propenyl (Allyl)						
71 DOE/TOS k_a . Pyrolysis in a Pyrex flask, in excess Toluene (as trapping agent for Allyl.) Gas-chromatography.	EX	694-759	1.07(12)	0	25667±403	1 1.82
76 SAK/NOH k_{overall} . Flow-reactor pyrolysis. Channel (a) proposed as first step of the overall reaction.	EX	773-893	7.94(12)	0	27680	1
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CD}_2 \rightarrow \text{CH}_2=\text{CHCH}_2\text{CD}_2\text{CH}=\text{CH}_2$ 1,5-Hexadiene-1,1-d ₂ → 1,5-Hexadiene-3,3-d ₂						
71 DOE/TOS Thermal isomerization in sealed ampoules. (Cope degenerated rearrangement.) Gas-chromatography.	EX	480-531	2.29(10)	0	17262	1
$\text{cis-CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow \text{trans-CH}_3\text{CH}=\text{C}(\text{CH}_3)\text{CH}=\text{CH}_2$ 1,3-Pentadiene, 3-methyl-, (Z)- → 1,3-Pentadiene, 3-methyl-, (E)-						
75 MAR/JEF Single-pulse shock-tube cis-trans isomerization in excess Ar. P(Ar) = (200-340) torr.	EX	955-1160	1.0(14)	0	27680±1007	1 2.0
$\text{CH}_2=\text{CHCH}(\text{CH}_3)\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2\text{CHCHCH}=\text{CH}_2 + \text{CH}_3$ 1,4-Pentadiene, 3-methyl-						
82 TRE Pyrolysis in a static system. Gas-chromatography. P = (15-200) torr.	EX	653-716	2.29(15)	0	32733±151	1 1.26
 → $\text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_2=\text{CH}_2$ Cyclohexene						
73 TSA1	EX	1050	1.41(15)	0	33500	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

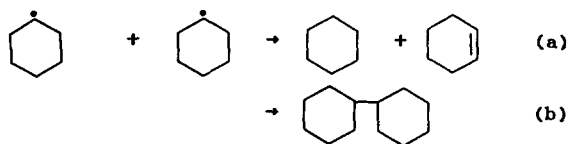
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 $\rightarrow \text{CH}_3\text{=CHCH}_2 + \text{CH}_2\text{=C=CH}_2$ (a) $\rightarrow \text{CH}_3\text{CH=C=CH}_2 + \text{CH}_2\text{=CH}_2$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{C(=CH}_2\text{)CH=CH}_2$ (c) \rightarrow  (d)						
Cyclobutane, ethylidene-						
\rightarrow 1-Propene + 1,2-Propadiene (Allene) (a)						
\rightarrow 1,2-Butadiene + Ethene (b)						
\rightarrow 1-Pentene, 3-methylene- (c)						
\rightarrow Cyclobutane, 1-methyl-2-methylene- (d)						
71 FLO/GIB1	EX	583-697	4.90(14)	0	31520±1432	1 8.51
k_a . Decyclization and decomposition.						
71 FLO/GIB1	EX	583-697	1.78(15)	0	31042±488	1 21.4
k_b . Decyclization and decomposition.						
71 FLO/GIB1	EX	583-697	1.20(13)	0	27504±2406	1 43.7
k_c . Isomerization by decyclization.						
71 FLO/GIB1	EX	583-697	8.32(13)	0	24801±503	1 2.29
k_d . Reversible rearrangement.						
Thermolysis in a static system.						
Gas-chromatography.						
Mass-spectrometry.						
 \rightarrow 						
Cyclobutane, 1-methyl-2-methylene-						
\rightarrow Cyclobutane, ethylidene-						
71 FLO/GIB1	EX	583-497	4.79(13)	0	24605±503	1 2.29
Thermolysis in a static system.						
Reversible rearrangement.						
Gas-chromatography.						
Mass-spectrometry.						
 $\rightarrow \text{CH}_2\text{=C(CH}_3\text{)CH}_2\text{CH=CH}_2$						
Cyclobutane, 1-methyl-3-methylene-						
\rightarrow 1,4-Pentadiene, 2-methyl-						
71 FLO/GIB2	EX	591-664	1.45(14)	0	26628±1661	1 14.1
Isomerization by decyclization.						
Thermolysis in a vacuum-system.						
Gas-chromatography.						
Mass-spectrometry.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}=\text{C}=\text{CH}_2$ (a)							
$\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_2=\text{C}=\text{CH}_2$ (b)							
\rightarrow  (c)							
\rightarrow  (d)							
\rightarrow  (e)							
Spiropentane, methyl-							
\rightarrow Ethene + 1,2-Butadiene (a)							
\rightarrow 1-Propene + 1,2-Propadiene (Allene) (b)							
\rightarrow Cyclobutane, ethylidene- (c)							
\rightarrow Cyclobutane, 1-methyl-2-methylene- (d)							
\rightarrow Cyclobutane, 1-methyl-3-methylene- (e)							
71 FLO/GIB2 ¹⁾	EX	591-664	3.02(15)	0	30003±608	1	2.63
k_a . Decyclization and decomposition.							
71 FLO/GIB2 ¹⁾	EX	591-664	2.09(15)	0	30093±841	1	3.89
k_b . Decyclization and decomposition.							
71 FLO/GIB2 ¹⁾	EX	591-664	1.38(14)	0	27084±209	1	1.41
k_c . Isomerization.							
71 FLO/GIB2 ¹⁾	EX	591-664	3.31(14)	0	27085±207	1	1.38
k_d . Isomerization.							
71 FLO/GIB2 ¹⁾	EX	591-664	2.40(14)	0	27085±209	1	1.41
k_e . Isomerization.							
71 FLO/GIB2 ¹⁾	EX	591-664	7.59(14)	0	27084±473	1	1.41
$k_a + k_b + k_c + k_d + k_e$. (Overall)							
¹⁾ Thermolysis in a static system. Gas-chromatography. Mass-spectrometry.							
$\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger \rightarrow \text{CH}_2\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$							
5-Hexenyl							
75 TAR ¹⁾	RL	298	8.95				1/1
k_{ref} :							
$(\text{CH}_3)_2\text{CCH}_2\text{CH}_3^\dagger \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3$							
75 TAR ¹⁾	RN	298	3.2(7)				1
¹⁾ $\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2^\dagger$ formed by: $\text{H} + \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2$.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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Cyclohexyl + Cyclohexyl

→ Cyclohexane + Cyclohexene (a)

→ 1,1'-Bicyclohexyl (b)

74 CUR/SID RL 360-460 (9.9±1.0)(-1) 0 0 2/2

k_a/k_b .

Azocyclohexane photolysis in a vacuum system.

Average ratio.

79 FUJ/GAE ¹⁾ RL 343-443 (5.6±0.1)(-1) 0 0 2/2

k_a/k_b .

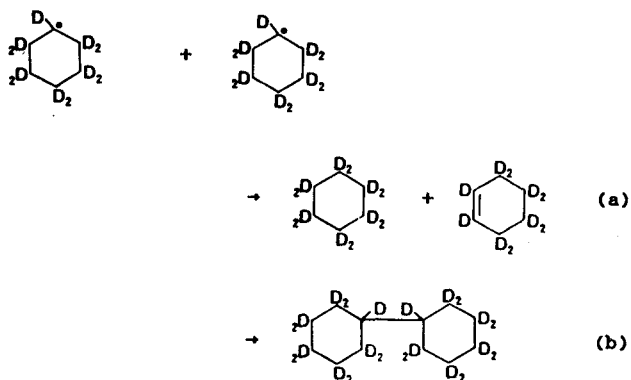
Assumed to be T-independent.

82 FUJ/GAE ¹⁾ RL 398-443 5.9(-1) 0 <500 2/2

k_a/k_b .

¹⁾ H₂O/Cyclohexane gas-phase radiolysis
in a Pyrex vessel.

P(Total) = (50-2400) torr.



Cyclohexyl-d₁₁ + Cyclohexyl-d₁₁

→ Cyclohexane-d₁₂ + Cyclohexene-d₁₀ (a)

→ 1,1'-Bicyclohexyl-d₂₂ (b)

79 FUJ/GAE ¹⁾ RL 343-473 (3.8±0.1)(-1) 0 0 2/2

k_a/k_b .

Assumed to be T-independent.

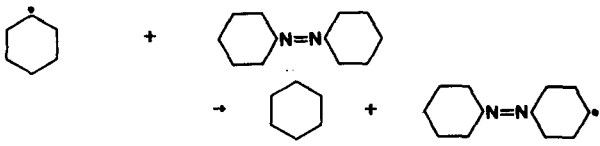
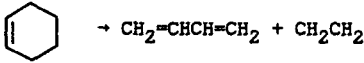
82 FUJ/GAE ¹⁾ RL 398-443 4.6(-1) 0 <500 2/2

k_a/k_b .



¹⁾ H₂O/Cyclohexane-d₁₂ gas-phase radiolysis
in a Pyrex vessel.

P(Total) = (50-2400) torr.


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 <p>Cyclohexyl + Diazene, dicyclohexyl- (Azocyclohexane)</p>	EX	360-460	3.98(8)	0	3322±503	2	1.26
74 CUR/SID Photolysis in a vacuum-system. Abstracted H assumed to be in position para to N=N group.							
$\text{CH}_2=\text{CH}(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{CH}_2=\text{CHCH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2$ (a) $\rightarrow \text{CH}_2=\text{CHCH}_3 + \text{CH}_2=\text{CHCH}_3$ (b)							
1-Hexene							
78 TSA5 ¹⁾ k_a . Bond-breaking reaction.	EX	990-1100	7.94(15)	0	35600±150	1	1.41
78 TSA5 ¹⁾ k_b . Molecular reaction.	EX	990-1100	3.98(12)	0	28900±200	1	1.58
¹⁾ 1-Hexene/Cyclohexene/Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the reaction:							
							
[1-Hexene] = 0.01%. [Toluene] = 1%. [Cyclohexene] = 0.01%. P(Ar) = 1.8 atm.							
79 KIN ²⁾ k_a . Bond-breaking reaction.	EX	915-1153	7.94(15)	0	35632±503	1	1.58
79 KIN ²⁾ k_b . Molecular reaction.	EX	915-1153	3.98(12)	0	29039±755	1	1.58
²⁾ Thermolysis using a VLPP technique.							
71 MAG/IOA k_{overall} .	EX	823-923	2.0(12)	0	25667	1	
$\text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 \rightarrow \text{trans-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3$							
2-Hexene, (Z)-							
74 BAU/YAD Rate-ratio assumed to be T-independent. k_{ref} : $\text{cis-CH}_3\text{CH}=\text{CHCH}_3 \rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3$	RL	1000-1150	1.0	0	0	1/1	
$(\text{CH}_3)_2\text{CHC}(\text{CH}_3)=\text{CH}_2 \rightarrow \text{CH}_3 + \text{CH}_3\text{CHC}(\text{CH}_3)=\text{CH}_2$							
1-Butene, 2,3-dimethyl-							
76 TSA1	ES	1080-1165	1.0(16)	0	35700	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_3\text{CCH}=\text{CH}_2 \rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CCH}=\text{CH}_2$ 1-Butene, 3,3-dimethyl-						
76 TSA1	ES	1080-1165	1.58(16)	0	35500	1
$\text{cis-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3 + \text{CH}_2=\text{CH}_2$ (a)						
 (b)						
$\rightarrow \text{trans-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ (c)						
1,4-Butanediyl, 1,2-dimethyl-, (Z)- \rightarrow 2-Butene, (Z)- + Ethene (a) \rightarrow Cyclobutane, 1,2-dimethyl, cis- (b) \rightarrow 1,4-Butanediyl, 1,2-dimethyl, (E)- (c)						
76 DER/UYE ¹⁾ k_a/k_b . Assumed to be T-independent.	RL	579-712	1.8	0	0	1/1
77 SCA/BAC ²⁾ k_b/k_a . Average ratio.	RL	663-703	(8.73±0.73)(-1)	0	0	1/1
77 SCA/RIC ³⁾ k_b/k_a .	RL	693	9.35(-1)			1/1
76 DER/UYE ¹⁾ k_b/k_c . Assumed to be T-independent.	RL	579-712	7.0(-1)	0	0	1/1
77 SCA/BAC ²⁾ $k_b/(k_a + k_b + k_c)$. Average ratio.	RL	663-703	(2.9±0.3)(-1)	0	0	1/1
77 SCA/BAC ²⁾ k_c/k_b . Average ratio.	RL	663-703	(1.36±0.10)	0	0	1/1
77 SCA/RIC ³⁾ k_c/k_b .	RL	693	1.38			1/1
¹⁾ Thermolysis. ²⁾ Average of four rate ratios in the given T-range. ³⁾ Calculated ratio. Static system. P = 12 atm.						
$\text{trans-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ $\rightarrow \text{trans-CH}_3\text{CH}=\text{CH}_3 + \text{CH}_2=\text{CH}_2$ (a)						
 (b)						
$\rightarrow \text{cis-CH}(\text{CH}_3)\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2$ (c)						
1,4-Butanediyl, 1,2-dimethyl-, (E)- \rightarrow 2-Butene, (E)- + Ethene (a) \rightarrow Cyclobutane, 1,2-dimethyl, trans- (b) \rightarrow 1,4-Butanediyl, 1,2-dimethyl, (Z)- (c)						
76 DER/UYE ¹⁾ k_a/k_b . Assumed to be T-independent.	RL	579-712	1.4	0	0	1/1

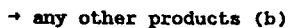
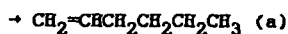
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
77 SCA/RIC ²) k _a /k _{ref} . k _{ref} : cis-CH(CH ₃)CH(CH ₃)CH ₂ CH ₂ → cis-CH ₃ CH=CHCH ₃ + CH ₂ =CH ₂	RL	693	(1.66±0.1)			1/1
77 SCA/BAC ³) k _b /k _a . Average ratio.	RL	663-703	(7.15±0.75)(-1)	0	0	1/1
77 SCA/RIC ²) k _b /k _a .	RL	693	6.6(-1)			1/1
77 SCA/BAC ³) k _b /(k _a + k _b + k _c). Average ratio.	RL	663-703	(3.23±0.15)(-1)	0	0	1/1
77 SCA/RIC ²) k _b /k _{ref} . k _{ref} : cis-CH(CH ₃)CH(CH ₃)CH ₂ CH ₂ → 	RL	693	(1.0±.01)			1/1
76 DER/UYE ¹) k _b /k _c . Assumed to be T-independent.	RL	579-712	1.9	0	0	1/1
77 SCA/BAC ³) k _c /k _b . Average ratio.	RL	663-703	(7.00±0.25)(-1)	0	0	1/1
77 SCA/RIC ²) k _c /k _b . Average ratio.	RL	693	7.15(-1)			1/1
77 SCA/BAC ³) k _c /k _{ref} . Average ratio. k _{ref} : cis-CH ₃ CHCH(CH ₃)CH ₂ CH ₂ → cis-CH ₃ CH=CHCH ₃ + CH ₂ =CH ₂	RL	663-703	(1.61±0.75)(-1)	0	0	1/1

1) Thermolysis.

2) Calculated ratios. Static system. P = 12 atm.

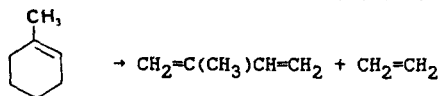
3) Average of four rate ratios in the given T-range.



Cyclohexane

78 TSA5 EX 990-1100 5.01(16) 0 44400±100 1 1.26

k_a. Cyclohexane/1-Methylcyclohexane/Ar
thermolysis in a single-pulse shock-tube.
k's determined relative to the reaction:






[1-Methylcyclohexene] = (0.002-0.005)%.

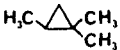
[Cyclohexane] = (0.4-1.0)%.

P(Ar) = (1.8-5.0) atm.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
73 ILL/WEL k_{overall} .	EX	825-1005	(2.15±0.12)(14)	0	32481	1
78 KAL/AND ¹⁾	RN	980	(2.5±0.5)(-1)			1
78 KAL/AND ¹⁾	RN	1028	(2.1±0.1)			1
¹⁾ k_{overall} . Cyclohexane/Hexane pyrolysis in a tubular reactor. In Hexane/Cyclohexane mixtures, the k of Cyclohexane decomposition increases when the initial [Hexane] decreases.						
79 KAL/NAM ²⁾ $k_{\text{overall}}/k_{\text{ref}}$. Average ratio. k_{ref} : CH ₃ CH ₃ → products.	RL	1033-1123	(8.4±1.3)	0	0	1/1
79 KAL/NAM ²⁾ $k_{\text{overall}}/k_{\text{ref}}$. Average ratio. k_{ref} : CH ₃ (CH ₂) ₄ CH ₃ → products.	RL	983-1133	(9.7±2.2)(-1)	0	0	1/1
79 KAL/NAM ²⁾ $k_{\text{overall}}/k_{\text{ref}}$.	RL	1153	1.9			1/1
k_{ref} :  → products.						
Rate ratio calculated from the ratio of other rate constants.						
²⁾ Cyclohexane/Ethane pyrolysis in a tubular reactor.						
 → trans-CH(CH ₃)CH(CH ₃)CH ₂ CH ₂						
Cyclobutane, 1,2-dimethyl-, trans- → 1,4-Butanediyl, 1,2-dimethyl-, (E)-						
77 SCA/BAC ¹⁾ Average ratio.	RL	663-703	(5.83±0.38)(-1)	0	0	1/1
77 SCA/RIC ¹⁾ Calculated ratio. Static system. P = 12 atm.	RL	693	(6.0±1.0)(-1)			1/1
¹⁾ k_{ref} :  → cis-CH(CH ₃)CH(CH ₃)CH ₂ CH ₂						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor	
 $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$ (a) $\rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}(\text{CH}_3)_2$ (b) $\rightarrow (\text{CH}_3)_2\text{C}=\text{CHCH}_2\text{CH}_3$ (c) $\rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}(\text{CH}_3)_2$ (d) $\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}(\text{CH}_3)_2$ (e) $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$ (f) $\rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2$ (g) \rightarrow other minor products (h)							
	Cyclopropane, 1,1,2-trimethyl-						
	\rightarrow 1-Pentene, 2-methyl-			(a)			
	\rightarrow 4-Pentene, 2-methyl-			(b)			
	\rightarrow 2-Pentene, 2-methyl-			(c)			
	\rightarrow 2-Pentene, 4-methyl-, (Z)-			(d)			
	\rightarrow 2-Pentene, 4-methyl-, (E)-			(e)			
	\rightarrow 1-Butene, 2,3-dimethyl-			(f)			
\rightarrow 2-Butene, 2,3-dimethyl-			(g)				
\rightarrow other minor products			(h)				
72 O'N/HEN 1)	EX	700-755	2.95(14)	0	30740±257	1	
$k_a + k_b + k_c + k_d + k_e + k_f + k_g + k_h$.							
Overall rate constant expression.							
72 O'N/HEN 1)	ES	700-755	7.76(13)	0	29693	1	
k_c .							
72 O'N/HEN 1)	ES	700-755	5.75(13)	0	30700	1	
k_d .							
72 O'N/HEN 1)	ES	700-755	1.35(14)	0	29693	1	
k_e .							
72 O'N/HEN 1)	ES	700-755	2.75(14)	0	29894	1	
$k_c + k_d + k_e$.							
72 O'N/HEN 1)	ES	700-755	1.26(14)	0	31002	1	
k_f .							
72 O'N/HEN 1)	ES	700-755	1.26(14)	0	31002	1	
k_g .							
72 O'N/HEN 1)	ES	700-755	2.51(14)	0	31002	1	
$k_f + k_g$.							
1) Thermolysis in a pyrex reaction-cell.							
Gas-chromatography.							
Overall rate constant determined experimentally.							
Rate constants for channels (a) through (g),							
or any combination of them, computed assuming							
a biradical mechanism and using transition							
state estimates of Arrhenius parameters							
(68 O'N BEN.)							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3^\dagger \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2$ Pentyl, 1-methyl- 75 TAR ¹⁾	RL	298	4.9(-1)			1/1
$k_{\text{ref}}: (\text{CH}_3)_2\text{CCH}_2\text{CH}_3^\dagger \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3$ 75 TAR ¹⁾	RN	298	1.8(6)			1
¹⁾ $\text{CH}_3\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ formed by: H + $\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$.						
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH} + \text{CH}_3\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3 + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (b) Butyl, 2,3-dimethyl- 75 BUL/MAR	RL	667-770	(5.56±0.11)(1)	0	0	1/1
k_a/k_b . Static system pyrolysis. Average ratio.						
$\text{CH}_3(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{products}$ (overall) Hexane 73 ILL/WEL P = 760 torr.	EX	870-1025	(2.34±0.05)(12)	0	26522	1
76 RYB/YAM M = Ar.	EX	973-1083	3.63(10)	0	23150	1
76 RYB/YAM M = D ₂ .	EX	973-1083	1.58(10)	0	22144	1
78 KAL/AVD ¹⁾	RL	980	(2.0±0.4)(1)			1/1
$k_{\text{ref}}: \text{C}_6\text{H}_{12} \rightarrow \text{products}$.						
78 KAL/AVD ¹⁾	RL	1028	(2.05±0.20)(1)			1/1
$k_{\text{ref}}: \text{C}_6\text{H}_{12} \rightarrow \text{products}$.						
78 KAL/AVD ¹⁾	RN	980	(5.0±1.0)			1
78 KAL/AVD ¹⁾	RN	1028	(4.3±0.2)(1)			1
¹⁾ Pyrolysis in a tubular reactor. In Hexane/Cyclohexane mixtures, the k of Cyclohexane decomposition increases when the initial [Hexane] decreases.						
79 KAL/NAM ²⁾	RL	1153	7.3			1/1
$k_{\text{ref}}: \text{CH}_3\text{CH}_3 \rightarrow \text{products}$.						
79 KAL/NAM ²⁾	RL	1153	1.29			1/1
$k_{\text{ref}}: \text{CH}_3(\text{CH}_2)_3\text{CH}_3 \rightarrow \text{products}$.						
²⁾ Pyrolysis of hydrocarbon mixtures in a tubular reactor. Calculated rate ratios.						

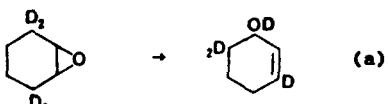
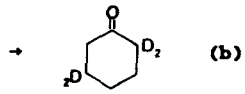
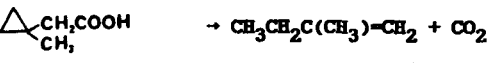
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	E, B-B(ref)	k, A units	k err. factor
80 RUM/SHE Pyrolysis in a quartz reactor. P = 760 torr.	EX	883-993	3.31(13)	0	30216±1311	1	3.89
$(\text{CH}_3)_2\text{CHCH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{products}$							
Pentane, 2-methyl-							
73 ILL/WEL P = 760 torr.	EX	853-1053	(1.03±0.03)(14)	0	29909	1	
$(\text{CH}_3)_3\text{CCH}_2\text{CH}_3 \rightarrow \text{products}$							
Butane, 2,2-dimethyl-							
73 ILL/WEL P = 760 torr.	EX	898-1053	(4.57±0.07)(13)	0	30191	1	
82 BIL/BAR Pyrolysis of 2,2-Dimethylbutane in a Pyrex vessel. Gas-chromatography. P = (50-150) torr.	EX	703-743	≈1.0(11)	0	25767	1	
$(\text{CH}_3)_3\text{CCH}_2\text{CH}_3 \uparrow \rightarrow \text{CH}_3 + (\text{CH}_3)_3\text{CCH}_2$ (a)							
$\rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CCH}_2\text{CH}_2$ (b)							
$\rightarrow \text{CH}_3\text{CH}_2 + (\text{CH}_3)_3\text{C}$ (c)							
Butane, 2,2-dimethyl-							
72 HAS/JOH ¹⁾ $k_a + k_b + k_c$. P = 0.017 torr.	EX	298	(4.6±0.8)(5)			1	
72 HAS/JOH ¹⁾ $k_a + k_b + k_c$. P = 0.033 torr.	EX	298	(8.7±1.2)(5)			1	
¹⁾ $(\text{CH}_3)_3\text{CCH}_2\text{CH}_3 \uparrow$ formed by $^1\text{CH}_2 + (\text{CH}_3)_4\text{C}$.							
$(\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH}$ (a)							
$\rightarrow \text{CH}_3 + (\text{CH}_3)_2\text{CHCHCH}_3$ (b)							
Butane, 2,3-dimethyl-							
74 GOL/ALF k_a . Best fit to experimental data to $\log A = 16.4$ for each C-C fission.	DE	990-1250	2.51(16)	0	37544	1	
75 BUL/MAR k_a . Static system pyrolysis.	ES	667-770	1.58(16)	0	37649	1	
78 TSA4 ¹⁾	EX	990-1100	1.58(16)	0	38100	1	
78 TSA4 ¹⁾ Extrapolation over the given T-range.	EX	300-1100	1.82(17)	0	40800	1	
¹⁾ k_a . Single-pulse shock-tube.							
75 BUL/MAR k_b . Static system pyrolysis.	ES	667-770	1.0(17)	0	40416	1	
75 BUL/MAR $k_a + k_b$. Static system pyrolysis.	ES	667-770	5.01(16)	0	38732	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
CH=CC(CH₃)₂COOH → CH₂=C=C(CH₃)₂ + CO₂							
3-Butynoic acid, 2,2-dimethyl-							
76 BIG/WEA1	EX	500	2.44(-5)			1	
76 BIG/WEA1	EX	500-630	1.79(11)	0	18266±758	1	
A and B recalculated from the reported data.							
CH₃C(O)OCH₂CH₂C≡CH → CH₃COOH + CH₂=CHC≡CH							
3-Butyn-1-ol acetate							
79 HER/CHU	EX	613-658	1.352(13)	0	23732±192	1	1.35
Pyrolysis in a static system. P = (53-180) torr.							
(CH₂=CHCH₂)₂O → CH₂=CHCHO + CH₃CH=CH₂							
1-Propene, 3,3'-oxybis- (Diallylether)							
→ 2-Propenal (Acrolein) + 1-Propene							
74 VIT/EGG3	EX	545-627	6.76(11)	0	20584±176	1	1.35
Pyrolysis in a static system. P = (4-84) torr.							
7-Oxabicyclo[4.1.0]heptane (1,2-Epoxycyclohexane)							
→ 2-Cyclohexen-1-ol (a)							
→ Cyclohexanone (b)							
→ other products (c)							
73 FLO/PEN1 ¹⁾	EX	680-740	1.29(13)	0	28082±654	1	2.57
k _a . P = (1.6-6) torr.							
74 FLO/PEN2 ¹⁾	EX	677-746	1.86(13)	0	28420±755	1	2.88
k _a . P = 4 torr.							
73 FLO/PEN1 ¹⁾	EX	680-740	3.80(14)	0	30347±554	1	2.24
k _b . P = (1.6-6) torr.							
74 FLO/PEN2 ¹⁾	EX	677-746	6.31(14)	0	30820±710	1	2.69
k _b . P = 4 torr.							
73 FLO/PEN1 ¹⁾	EX	677-736	1.38(14)	0	29190±554	1	2.19
k _a + k _b + k _c .							
P = (1.6-6) torr.							
74 FLO/PEN2 ¹⁾	EX	677-746	2.29(14)	0	29653±846	1	3.31
k _a + k _b + k _c .							
P = 4 torr.							
¹⁾ Thermolysis in a static system.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
  other products (c)							
7-Oxabicyclo[4.1.0]heptane-2,2,5,5-d ₄ (1,2-Epoxy-cyclohexane-2,2,5,5-d ₄)							
→ 2-Cyclohexen-3,6,6-d ₃ -ol-d (a)							
→ Cyclohexanone-2,2,5,5-d ₄ (b)							
→ other products (c)							
74 FLO/PEN2 ¹⁾ k _a . P = 4 torr.	EX	677-746	2.19(13)	0	29225±493	1	2.0
74 FLO/PEN2 ¹⁾ k _b . P = 4 torr.	EX	677-746	7.24(14)	0	30951±523	1	2.09
74 FLO/PEN2 ¹⁾ k _a + k _b + k _c . P = 4 torr.	EX	677-746	4.47(14)	0	30398±760	1	2.88
¹⁾ Thermolysis in a static system.							
CH ₂ =C=C(CH ₃) ₂ COOH → CH ₂ =C=C(CH ₃) ₂ + CO ₂ 3-Butenoic acid, 2,2-dimethyl-							
82 ALB/BIG ¹⁾	EX	577	9.7(-4)				1
82 ALB/BIG ¹⁾	EX	~577	1.03(11)	0	18619		1
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a flow-reactor. NMR-spectrometry.							
CH ₃ C(O)OCH ₂ CH ₂ CH=CH ₂ → CH ₃ COOH + CH ₂ =C=C(CH ₃)=CH ₂ 3-Buten-1-ol acetate							
79 MAR/HER	EX	513-693	1.58(13)	0	24153±253	1	1.48
Pyrolysis in a static system. Gas-chromatography. P = (44-282) torr.							
 Cyclopropaneacetic acid, 1-methyl- → 1-Propene, 2-methyl- + Carbon dioxide							
79 BIG/FET ¹⁾	EX	725	(8.24±0.35)(-2)				1
79 BIG/FET ¹⁾	EX	690-740	(4.62±0.20)(11)	0	21282±1311		1
A and B recalculated from the reported data.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
1) Pyrolysis in a Flow-reactor with evacuated sealed tubes. Gas-chromatography. NMR-spectroscopy.							
$\begin{array}{c} \text{H}_3\text{C} \\ \diagdown \\ \text{CH}_2\text{COOH} \end{array}$			$\rightarrow (\text{CH}_3)_2\text{CHCH}=\text{CH}_2 + \text{CO}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 + \text{CO}_2$ (b) $\rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CO}_2$ (c)				
Cyclopropaneacetic acid, 2-methyl-, trans-							
			\rightarrow 1-Butene, 3-methyl- + Carbon dioxide (a)				
			\rightarrow 1-Pentene + Carbon dioxide (b)				
			\rightarrow 1-Butene, 2-methyl- + Carbon dioxide (c)				
80 BIG/FET ¹⁾	EX	725	1.13(-3)				1
k_a .							
80 BIG/FET ¹⁾	EX	725	5.7(-4)				1
k_b .							
80 BIG/FET ¹⁾	EX	725	<4.0(-5)				1
k_c . Upper-limit k.							
80 BIG/FET ¹⁾	EX	725	1.7(-3)				1
$k_a + k_b + k_c$.							
80 BIG/FET ¹⁾	EX	750-820	3.31(11)	0	23855±601		1
$k_a + k_b + k_c$.							
A and B recalculated from the reported data.							
1) Pyrolysis in a flow-reactor with evacuated sealed tubes. Gas-chromatography. NMR-spectrometry.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_3\text{C}(\text{O})\text{CH}=\text{CH}_2$ 2-Butanone, 4-(acetyloxy)-							
72 TIN/KOO	EX	587-636	7.94(12)	0	18520±503	1	2.51
Thermolysis.							
$(\text{CH}_3)_2\text{CHCH}_2\text{OCH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CH}_3\text{CHO}$ Propane, 1-(ethenyloxy)-2-methyl-							
74 BAM	EX	653-708	3.80(10)	0	20990±120	1	1.20
Thermolysis in a static system.							
Gas-chromatography.							
$(\text{CH}_3)_2\text{CHOC}(\text{CH}_3)=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CO} + \text{CH}_3\text{CH}=\text{CH}_2$ 1-Propene, 2-(1-methylethoxy)-							
81 FLO/HON	EX	554-613	9.55(11)	0	20220±613	1	2.88
Thermolysis in a static system.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_3\text{COCH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CHO} + (\text{CH}_3)_2\text{C}=\text{CH}_2$ Propane, 2-(ethenyloxy)-2-methyl- 79 ROS/GOL VLP-Pyrolysis. High-pressure k. RRKM best data-fit.	EX	625-925	1.0(12)	0	19326±503	1	1.86
$\text{H}_3\text{C}-\text{CH}_2-\text{C} \begin{array}{l} \diagup \text{O} \\ \diagdown \end{array} \text{CH}_3 \rightarrow \text{HCHO} + \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ Oxetane, 3-ethyl-3-methyl- 75 CLE/FRE Thermolysis in a static system.	EX	680-721	2.28(15)	0	30219±243	1	1.42
$\text{H}_3\text{C} \begin{array}{l} \diagup \text{O} \\ \diagdown \end{array} \text{C}(\text{CH}_3)_2 \begin{array}{l} \diagup \text{CH}_3 \\ \diagdown \end{array} \rightarrow \text{CH}_3\text{COC}(\text{CH}_3)_3 \quad (\text{a})$ $\rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)_2\text{OH} \quad (\text{b})$ $\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{CO} \quad (\text{c})$ Oxirane, tetramethyl- \rightarrow 2-Butanone, 3,3-dimethyl- (a) \rightarrow 1-Buten-3-ol, 2,3-dimethyl- (b) \rightarrow 1-Propene + 2-Propanone (c)	EX	642-733	3.72(13)	0	28074±746	1	2.88
81 FLO/HON ¹⁾ k_a .	EX	642-733	6.46(11)	0	25236±1504	1	8.71
81 FLO/HON ¹⁾ k_b .	EX	642-733	3.55(13)	0	28267±541	1	2.19
81 FLO/HON ¹⁾ k_c . ¹⁾ Thermolysis in a static system.	EX	642-733	3.55(13)	0	28267±541	1	2.19
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$ Acetic acid butyl ester (n-Butyl acetate) 72 TIN/KOO Thermolysis.	EX	668-741	2.51(12)	0	23805±252	1	1.58
76 DEB/TAY	EX	650-700	3.98(12)	0	24207	1	
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Propanoic acid 1-methylethyl ester 77 CHU/MAR 77 SMI/MUT	EX	563-623	1.15(13)	0	22849±101	1	1.23
	EX	651	(6.10±0.20)(-3)			1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$							
Acetic acid 1,1-dimethylethyl ester (t-Butyl acetate)							
75 TAY ¹⁾	EX	557-609	2.0(13)	0	20282±176	1	1.26
78 AMI/TAY1 ¹⁾	EX	518-609	1.15(13)	0	199975	1	
¹⁾ Pyrolysis in a stainless-steel reactor.							
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CD}_3)_3 \rightarrow \text{CH}_3\text{COOD} + (\text{CD}_3)_2\text{C}=\text{CD}_2$							
Acetic acid 1,1-dimethylethyl-d ₉ ester (t-Butyl-d ₉ acetate)							
78 AMI/TAY1	EX	558-608	2.4(13)	0	20921	1	
Pyrolysis in a stainless-steel reactor.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{OCH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{OCH}_3$							
1-Propanol, 3-methoxy-, acetate							
76 DEB/TAY	EX	650,700	4.47(12)	0	24409	1	
$\text{CH}_3\text{OCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{OCH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Acetic acid, methoxy-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.87±0.27)(-3)			1	
78 CHU/MAR ¹⁾	EX	603	5.89(-4)			1	
78 CHU/MAR ¹⁾	EX	583-633	1.10(13)	0	22597±151	1	1.35
¹⁾ Pyrolysis in a static system.							
$\text{CH}_3\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_3$							
→ $\text{CH}_2=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$ (a)							
→ $\text{CH}_3\text{CH}_2\text{OH} + \text{CO}_2 + \text{CH}_3\text{CH}=\text{CH}_2$ (b)							
Carbonic acid ethyl propyl ester (Ethyl propyl carbonate)							
76 CRO/HUN	EX	581-664	7.76(11)	0	21843	1	
$k_a + k_b$.							
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CO}$ (a)							
→ $(\text{CH}_3)_2\text{CHCOCH}_3 + \text{CH}_3$ (b)							
Propoxy, 1,1,2-trimethyl-							
75 ALC/MIL	ES	373	4.7(6)			1	
k_a .							
75 ALC/MIL	ES	373	1.5(8)			1	
k_b .							
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 + \text{O}_2 \rightarrow \text{products}$							
Propoxy, 1,1,2-trimethyl- + Oxygen molecule							
75 ALC/MIL	ES	373	1.2(9)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$(\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ $\rightarrow (\text{CH}_3)_2\text{CHCH}(\text{OH})(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2$ Propoxy, 1,1,2-trimethyl- + Butane, 2,3-dimethyl- 75 ALC/MIL	ES	373	4.0(8)			2
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHCH}(\text{CH}_3)_2$ $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{OOH})(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2$ Propylldioxy, 1,1,2-trimethyl- + Butane, 2,3-dimethyl 75 ALC/MIL	ES	373	1.6(5)			2
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 + (\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2$ $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2$ $+ (\text{CH}_3)_2\text{CHC}(\text{O}\cdot)(\text{CH}_3)_2 + \text{O}_2$ (a) \rightarrow Fragmentation products (b) Propylldioxy, 1,1,2-trimethyl- 75 ALC/MIL k_a .	ES	373	2.3(11)			2
75 ALC/MIL k_b .	ES	373	2.4(11)			2
$(\text{CH}_3)_2\text{CHC}(\text{OO}\cdot)(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHC}(\text{O})\text{CH}_3 + \text{CH}_3$ (a) $\rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CO}$ (b) Propylldioxy, 1,1,2-trimethyl- 77 ALC/MIL ¹⁾	RN	373	1.5(8)			1
k_a . (α -scission). Estimated k. 77 ALC/MIL ¹⁾	RN	373	4.7(6)			1
k_b . (β -scission). Estimated k. ¹⁾ Azomethane photolysis.						
$(\text{CH}_3)_2\text{CHC}(\text{CH}_3)_2\text{OH} \rightarrow (\text{CH}_3)_2\text{CH} + \text{C}(\text{CH}_3)_2\text{OH}$ (a) $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{CH}_3)=\text{CH}_2 + \text{H}_2\text{O}$ (b) $\rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{H}_2\text{O}$ (c) 2-Butanol, 2,3-dimethyl- 76 TSA1	EX	1080-1165	1.74(16)	0	37400	1
k_a .	EX	1080-1165	1.48(14)	0	32300	1
k_b .	EX	1080-1165	4.57(13)	0	32700	1
k_c .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{OH} \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3\text{CHOH}$ (a) $\rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}_2 + \text{H}_2\text{O}$ (b)							
2-Butanol, 3,3-dimethyl-							
76 TSA1 k_a .	EX	990-1125	2.14(16)	0	37500	1	
76 TSA1 k_b .	EX	990-1125	<1.0(14)	0	34200	1	
Upper-limit k.							
$\text{CH}_2=\text{CHCH}_2\text{SCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCHS} + \text{CH}_3\text{CH}=\text{CH}_2$ 1-Propene, 3,3'-thiobis- (Diallyl sulfide) \rightarrow 2-Propenethial + 1-Propene							
82 MAR/ROP2 Pyrolysis in a stirred-flow system. 2-Propenethial (Thioacrolein) polymerizes into a film. Mass-spectrometry. P = (2-15) torr.	EX	588-691	1.02(11)	0	16960±84	1	1.15
$\text{CH}_3\text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CHS} + \text{CH}_3\text{CH}=\text{CH}_2$ 1-Propene, 3-(propenylthio)- \rightarrow Propanethial + 1-Propene							
82 MAR/ROP1 ¹⁾	EX	543-673	3.31(11)	0	18885±241	1	1.45
82 MAR/ROP1 ¹⁾ Alternate expression, including the previous (static) and the present (flow) measurements. ¹⁾ Pyrolysis in a static system. Mass- and NMR- spectrometry. Propanethial trimerizes into the cyclic compound: 2,4,6-Triethyl-1,3,5-trithiane. P(Total) =(2-18) torr.	SE	535-680	1.15(11)	0	18355±352	1	1.15
$\text{CH}_3\text{C}(\text{S})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3 \rightarrow \text{CH}_4 + \text{COS} + \text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2$ (a) $\rightarrow \text{CH}_3\text{C}(\text{O})\text{SCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (b)							
Ethanethioic acid O-butyl ester							
75 BIG/GAB ¹⁾ k_a . Elimination.	EX	635	2.16(-2)			1	
75 BIG/GAB ¹⁾ k_a . Elimination.	EX	613-641	2.51(12)	0	20382	1	
75 BIG/GAB ¹⁾ k_b . Isomerization.	EX	629	2.86(-3)			1	
75 BIG/GAB ¹⁾ k_b . Isomerization.	EX	613-641	7.94(11)	0	20886	1	
75 BIG/GAB ¹⁾ $k_a + k_b$. Overall reaction.	EX	633	2.97(-2)			1	


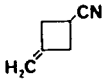
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
75 BIG/GAB $k_a + k_b$. Overall reaction. 1) Flow-reactor pyrolysis.	EX	613-641	1.26(12)	0	19829	1
CH₃C(S)OCH(CH₃)CH₂CH₃						
→ CH ₄ + COS + cis-CH ₃ CH=CHCH ₃ (a)						
→ CH ₄ + COS + trans-CH ₃ CH=CHCH ₃ (b)						
→ CH ₄ + COS + CH ₂ =CHCH ₂ CH ₃ (c)						
Ethanethioic acid O-(1-methylpropyl) ester						
75 BIG/GAB 1)	EX	571	3.4(-2)			1
75 BIG/GAB 1)	EX	629	7.33(-1)			1
75 BIG/GAB 1)	EX	545-575	2.51(12)	0	18218	1
1) $k_a + k_b + k_c$. Elimination. Flow-reactor pyrolysis. Probably isomerization not occurring.						
CH₃C(S)OCH₂CH(CH₃)₂ → CH₄ + COS + (CH₃)₂C=CH₂ (a)						
→ CH ₃ C(O)SH ₂ CH(CH ₃) ₂ (b)						
Ethanethioic acid O-(2-methylpropyl) ester						
75 BIG/GAB 1)	EX	629	1.30(-2)			1
k_a . Elimination.						
75 BIG/GAB 1)	EX	623-657	3.55(12)	0	20936	1
k_a . Elimination.						
75 BIG/GAB 1)	EX	629	2.49(-3)			1
k_b . Isomerization.						
75 BIG/GAB 1)	EX	649	4.38(-2)			1
$k_a + k_b$. Overall reaction.						
75 BIG/GAB 1)	EX	623-657	1.58(12)	0	20232	1
$k_a + k_b$. Overall reaction. 1) Flow-reactor pyrolysis.						
CH₃C(O)SCH₂CH₂CH₂CH₃ → CH₄ + COS + CH₂=CHCH₂CH₃						
Ethanethioic acid S-butyl ester						
73 BIG/GAB 1)	EX	790	3.0(-2)			1
73 BIG/GAB 1)	EX	780-810	3.98(11)	0	23402±453	1
1) Elimination. Flow-reactor pyrolysis.						
CH₃C(O)SCH₂CH(CH₃)₂ → CH₄ + COS + (CH₃)₂C=CH₂						
Ethanethioic acid S-(2-methylpropyl) ester						
73 BIG/GAB 1)	EX	804	3.3(-2)			1
73 BIG/GAB 1)	EX	790-825	6.31(11)	0	24660±755	1
1) Elimination. Flow-reactor pyrolysis.						

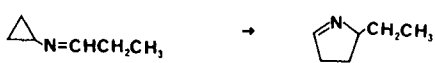

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃C(O)SCH(CH₃)CH₂CH₃						
→ CH ₄ + COS + cis-CH ₃ CH=CHCH ₃ (a)						
→ CH ₄ + COS + trans-CH ₃ CH=CHCH ₃ (b)						
→ CH ₄ + COS + CH ₂ =CHCH ₂ CH ₃ (c)						
Ethanethioic acid S-(1-methylpropyl) ester						
73 BIG/GAB ¹⁾	EX	730	3.2(-2)			1
73 BIG/GAB ¹⁾	EX	714-743	5.01(11)	0	22144±504	1
¹⁾ k _a + k _b + k _c . Elimination. Flow-reactor pyrolysis.						
CH₃C(O)SC(CH₃)₃ → CH₄ + COS + (CH₃)₂C=CH₂						
Ethanethioic acid S-(1,1-dimethylethyl) ester						
72 OEL/TIN	EX	653-705	6.31(13)	0	23000	1
Elimination by thermolysis.						
73 BIG/GAB ¹⁾	EX	652	1.8(-2)			1
73 BIG/GAB ¹⁾	EX	650-680	1.58(12)	0	20936±201	1
¹⁾ Elimination. Flow-reactor pyrolysis.						
CH₃OC(O)SC(CH₃)₃ → CH₃OH + C(O)S + CH₂=C(CH₃)₂						
Carbonothioic acid S-(1,1-dimethylethyl) O-methyl ester						
79 ALA/BIG ¹⁾	EX	629	1.2(-3)			1
79 ALA/BIG ¹⁾	EX	643-693	1.35(12)	0	21799±722	1
A and B recalculated from the reported data. ¹⁾ Flow-reactor pyrolysis. (Flow-tube method.)						
(CH₃)₃COC(O)SCH₃ → (CH₃)₂C=CH₂ + CO₂ + CH₃SH						
Carbonothioic acid O-(1,1-dimethylethyl) S-methyl ester						
79 ALA/BIG ¹⁾	EX	629	4.2(-4)			1
79 ALA/BIG ¹⁾	EX	752-775	4.88(10)	0	16025±203	1
A and B recalculated from the reported data. ¹⁾ Flow-reactor pyrolysis. (Inhibited tube method.)						
CH₃C(S)SCH₂CH₂CH₂CH₃ → CH₄ + CS₂ + CH₂=CHCH₂CH₃						
Ethane(dithioic) acid butyl ester						
78 ALA/BIG ¹⁾	EX	629	3.3(-3)			1
78 ALA/BIG ¹⁾	EX	651-716	1.08(13)	0	22473	1
A and B recalculated from the reported data. ¹⁾ Flow-reactor pyrolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{S})\text{SCH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{cis-CH}_3\text{CH}=\text{CHCH}_3$ (a)						
$\rightarrow \text{trans-CH}_3\text{CH}=\text{CHCH}_3$ (b)						
$\rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}_3$ (c)						
Ethane(dithioic) acid 1-methylpropyl ester						
78 ALA/BIG ¹⁾	EX	629	7.4(-2)			1
78 ALA/BIG ¹⁾	EX	584-639	6.67(12)	0	22211	1
A and B recalculated from the reported data.						
¹⁾ $k_a + k_b + k_c$.						
Pyrolysis in a flow-reactor.						
$\text{CH}_3\text{C}(\text{S})\text{SC}(\text{CH}_3)_3 \rightarrow \text{CH}_4 + \text{CS}_2 + \text{CH}_2=\text{C}(\text{CH}_3)_2$						
Ethane(dithioic) acid 1,1-dimethylethyl ester						
78 ALA/BIG ¹⁾	EX	629	3.1(-1)			1
78 ALA/BIG ¹⁾	EX	448-502	1.05(13)	0	19598	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow-reactor.						
$\text{CH}_3\text{OC}(\text{S})\text{SC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{OH} + \text{CS}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$						
Carbonodithioic acid S-(1,1-dimethylethyl) O-methyl ester						
82 ALA/BIG ¹⁾	EX	629	4.3(-1)			1
82 ALA/BIG ¹⁾	EX	540-570	1.90(11)	0	16867	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a flow reactor.						
IR-spectrometry.						
P = (2-800) torr.						
						
$\rightarrow \text{CH}_2=\text{CHCN} + \text{CH}_2=\text{CHCN}$						
1,2-Cyclobutanedicarbonitrile, trans-						
72 SAR/GAL	EX	726-783	2.51(12)	0	20735	1
Thermolysis in a flow-reactor.						
Gas-chromatography.						
						
$\rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_2=\text{CHCN}$						
1-Cyclobutanecarbonitrile, 3-methylene-						
72 SAR/GAL ¹⁾	EX	726-783	5.01(12)	0	24711	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 SAR/GAL ¹⁾ Average between the previous and present data.	SE	726-783	5.27(12)	0	24711	1
¹⁾ Thermal isomerization in a flow-reactor. Gas-chromatography.						
						
Cyclopropanamine, N-propylidene- → 2H-Pyrrole, 2-ethyl-3,4-dihydro- (5-Ethyl-1-pyrroline)						
72 COC/EGG1 Thermolysis in a static system. Gas-chromatography. P-independent k from 2.5 to 55 torr.	EX	573-635	1.12(14)	0	24041±81	1 1.15
						
2H-Pyrrole, 2-ethyl-3,4-dehydro- (5-Ethyl-1-pyrroline) → 3H-Pyrrole, 2-ethyl- + Hydrogen molecule						
72 COC/EGG2 Pyrolysis in a static system. Gas-chromatography. P = (12-60) torr.	EX	721-786	3.16(12)	0	27932±700	1 2.51
$\text{CH}_2=\text{CHCH}_2\text{NHCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CH}_2=\text{CHCH}=\text{NH}$						
2-Propen-1-amine, N-(2-propenyl)-						
74 EGG/VIT1	EX	533-616	1.10(11)	0	18676±166	1 1.35
$(\text{CH}_3)_2\text{CHN}=\text{NCH}_2\text{CH}=\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH} + \text{CH}_2\text{CH}=\text{CH}_2 + \text{N}_2$						
Diazene, (1-methylethyl)-2-propenyl-						
72 CRA/TAK Thermolysis. Gas-chromatography. Mass-spectrometry. In presence of ¹⁵ NO. P(Total) = (50-60) torr.	EX	374-399	6.31(14)	0	17916±252	1 1.91

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

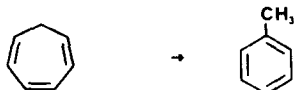
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A	k err. units factor
$\text{CH}_3\text{CH}_2\text{CH}_2\text{N}=\text{NCH}_2\text{CH}_2\text{CH}_3^* \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2 + \text{CH}_3\text{CH}_2\text{CH}_2 + \text{N}_2$							
Diazene, dipropyl- (Azo-n-propane)							
77 CHE/ORE Azo-n-propane/He high-pressure photolysis. RRKM data-fit on the basis of a proposed mechanism. Azon-propane assumed to be in vibrationally excited T_1 electronic state. Lower-limit k. $P(\text{CO}_2) = (0-45)$ atm. $P(\text{He}) = (0-50)$ atm.	EX	298	4.0(7)			1	
81 ADA/BAS1 Flash-photolysis in N_2 . Kinetic spectroscopy.	EX	298	(6.6±1.3)(7)			1	
$(\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} + \text{N}_2$							
Diazene, bis(1-methylethyl)- (Azoisopropane)							
73 PER/BEA RRKM fit of experimental data.	EX	625-830	3.98(16)	0	24107±503	1	
77 MCK/TUR ¹⁾ Series A Pyrolysis.	EX	503-544	2.04(16)	0	23956±849	1	4.90
77 MCK/TUR ¹⁾ Series B Pyrolysis.	EX	518-573	2.14(17)	0	25437±309	1	1.74
¹⁾ Static system thermolysis.							
79 SZI Static system thermolysis.	EX	494-446	3.98(14)	0	21411±481	1	2.51
80 ACS/PET Thermolysis in a high-vacuum system.	EX	523-623	1.58(16)	0	23672±313	1	2.0
82 MCM/LEW ²⁾ Experimental rate expression.	EX	780-1025	3.24(13)	0	19930±503	1	1.12
82 MCM/LEW ²⁾ Best fit to present and previous data.	SE	780-1025	7.94(13)	0	20735	1	
²⁾ Laser-powered homogeneous pyrolysis in excess Toluene, or Cumene as scavengers.							
$(\text{CH}_3)_2\text{CHN}=\text{NCH}(\text{CH}_3)_2^* \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{CH} + \text{N}_2$							
Diazene, bis(1-methylethyl)- (Azoisopropane)							
77 CHE/ORE Azoisopropane/He high-pressure photolysis. RRKM data-fit on the basis of a proposed mechanism. Azoisopropane is assumed to be in a vibrationally excited T_1 electronic state. Lower-limit k. $P(\text{CO}_2) = (0-45)$ atm. $P(\text{He}) = (0-100)$ atm.	EX	298	5.0(8)			1	
81 ADA/BAS1 Flash-photolysis in N_2 . Kinetic spectroscopy.	EX	298	(1.6±0.4)(8)			1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{CONHC}(\text{CH}_3)_3 (+ \text{M}) \rightarrow \text{CH}_3\text{CONH}_2 + (\text{CH}_3)_2=\text{CH}_2 (+ \text{M})$ (a) $\rightarrow \text{CH}_2=\text{C}=\text{O} + (\text{CH}_3)_3\text{CNH}_2 (+ \text{M})$ (b)							
Acetamide, N-(1,1-dimethylethyl)- → Acetamide + 1-Propene, 2-methyl- (a) → Ethenone + 2-Propanamine, 2-methyl- (b)							
73 MAC/NAG ¹⁾ k _a . Six-centered transition state assumed.	EX	658-738	2.63(12)	0	25939±533	1	2.14
73 MAC/NAG ¹⁾ k _b . M = CH ₃ COOH.	EX	673-725	3.63(13)	0	17589±644	2	2.51
¹⁾ Vacuum-system pyrolysis. P-independent k within the given P-range. Acetic acid catalysis. P = (52-412) torr.							
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CN} \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}(\text{CH}_3)\text{CN}$							
Propanenitrile, 2-(acetyloxy)-2-methyl- 80 MAR/CHU Static system pyrolysis. Mass-spectrometry. IR-, and NMR-spectroscopy. P = (56-210) torr.	EX	503-613	2.82(14)	0	23901±1059	1	6.61
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{N}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHN}(\text{CH}_3)_2$							
Acetic acid 2-(dimethylamino)ethyl ester 80 CHU/MAR Pyrolysis in a static system. Gas-chromatography. P = (63-207) torr.	EX	592-723	7.94(13)	0	6511±457	1	2.0
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{NH} + \text{CO}_2 + \text{CH}_3\text{CH}=\text{CH}_2$							
Carbamic acid, dimethyl-, 1-methylethyl ester 72 DAL/ZIO2 Pyrolysis in a conventional static system.	EX	323-333	1.10(13)	0	21797±201	1	
$\text{CH}=\text{CCH}_2\text{CH}_2\text{CH}_2\text{C}\equiv\text{CH} \rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_2=\text{CHC}\equiv\text{CH}$							
1,6-Heptadiyne 80 KIN VLP-Pyrolysis. High-pressure k extrapolated from VLPP data by means of RRKM theory.	EX	794-1225	3.98(12)	0	26019±503	1	2.51
$\text{CH}_2=\text{C}=\text{CHCH}(\text{CH}_3)\text{C}\equiv\text{CH} \rightarrow \text{CH}=\text{CCH}_2\text{CH}=\text{C}=\text{CCH}_3$							
1,2-Hexadien-5-yne, 4-methyl- 72 HOP	EX	423-473	6.92(10)	0	15501±151	1	1.35

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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1,3,5-Cycloheptatriene → Benzene, methyl- (Toluene)

75 LUU/GLA ¹⁾	EX	900-1300	3.16(13)	0	25140±722	1 1.58
75 LUU/GLA ¹⁾	SE	600-1300	6.31(13)	0	26222±120	1 1.12

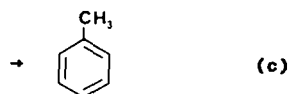
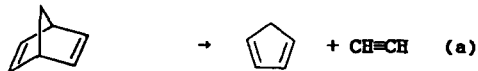
Extended Arrhenius expression over the low and high T-range, by combining the previous and the present data.

¹⁾ M = Ar. Thermal isomerization behind incident and reflected shock-waves.

Total Conc. = (0.6-6.0) × 10¹⁸ molec. cm⁻³.

[Cycloheptatriene] = (0.01-1.0)%

P-independent k.



Bicyclo[2.2.1]hepta-2,5-diene

(2,5-Norbornadiene)

→ 1,3-Cyclopentadiene + Ethyne (a)

→ 1,3,5-Cycloheptatriene (b)

→ Benzene, methyl- (Toluene) (c)

75 WAL/WEL ¹⁾	EX	584-630	6.03(14)	0	25853±146	1 1.26
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k_a.

Decomposition.

75 WAL/WEL ¹⁾	EX	584-630	7.94(14)	0	25848±151	1 1.29
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k_b + k_c.

Isomerization by ring expansion and by rearrangement.

¹⁾ Decomposition in a static vacuum system.







Bicyclo[2.2.1]hept-2-ene (Norbornene)

→ 1,3-Cyclopentadiene + Ethene

76 WAL/WEL	EX	521-570	1.8(14)	0	22420±360	1 1.9
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Decomposition of Norbornene in a static system.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 →  (a)							
→  + CH ₂ =CH ₂ (b)							
→ cis-CH ₂ =CHCH=CHCH=CHCH ₃ → products (c)							
Bicyclo[3.2.0]hept-2-ene							
→ -Bicyclo[2.2.1]hept-2-ene (Norbornene) (a)							
→ 1,3-Cyclopentadiene + Ethene (b)							
→ 1,3,6-Heptatriene, (Z)- → products (c)							
71 COC/FREZ ¹⁾ k _a . Isomerization.	ES	580-626	2.24(11)	0	21062±528	1	2.40
71 COC/FREZ ¹⁾ k _b . Decomposition.	ES	580-626	7.94(15)	0	26850±453	1	2.14
71 COC/FREZ ¹⁾ k _{overall} . Isomerization by decyclization.	ES	580-626	3.16(12)	0	23150±1812	1	2.0
The products formed by further isomerization are believed to be:							
1-Methyl-1,3-Cyclohexadiene,							
2-Methyl-1,3-Cyclohexadiene,							
5-Methyl-1,3-Cyclohexadiene,							
1,3,5-Heptatriene, (E,E)- (trans,trans)							
1,3,5-Heptatriene, (Z,Z)- (cis,cis).							
71 COC/FREZ ¹⁾ k _a + k _b .	EX	580-626	7.08(14)	0	25174±302	1	1.62
71 COC/FREZ ¹⁾ k _{overall} .	EX	580-626	5.75(14)	0	24979±121	1	1.23
1) Pyrolysis in a conventional static system. Gas-chromatography. The k's for the channels (a), (b) and (c), subject to errors, are given with caution. P = torr.							
 → CH ₂ =C=CHCH ₂ CH ₂ CH=CH ₂ (a)							
→ CH ₂ =CHC(=CH ₂)CH ₂ CH=CH ₂ (b)							
Tricyclo[4.1.0.0^{1,3}]heptane							
→ 1,2,6-Heptatriene (a)							
→ 1,5-Hexadiene, 3-methylene- (b)							
71 FRE/HOP ¹⁾ k _a .	EX	423-463	1.2(14)	0	18740±332	1	2.14

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k(k(ref)), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
71 FRE/HOP ¹⁾ k _b . 1) Thermal isomerization in a static system. k is P-independent within the (0.2-2.3) torr. range. Gas-chromatography.	EX	423-463	1.62(14)	0	17898±126	1	1.32
$\text{CH}\equiv\text{CCH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_3 \rightarrow \text{CH}\equiv\text{CCH}_2 + \text{CH}_3\text{CHCH}_2\text{CH}_3 \quad (\text{a})$ $\rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_3 \quad (\text{b})$							
1-Hexyne, 4-methyl-							
78 TSA3 ¹⁾ k _a . Bond-breaking reaction.	EX	990-1200	7.94(15)	0	35000±500	1	1.58
78 TSA3 ¹⁾ k _b . Molecular reaction.	EX	990-1200	7.94(12)	0	28000±1000	1	2.51
¹⁾ 4-Methyl-1-hexyne/Cyclohexene/Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexane. Similar data given 76 TSA2. [4-Methyl-1-hexyne] = 0.02%. [Cyclohexene] = 0.01%. P(Ar) ~ (2-6) atm. [Toluene] = 1%.							
$\text{CH}\equiv\text{CCH}_2\text{CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{CH}\equiv\text{CCH}_2 + \text{CH}_2\text{CH}(\text{CH}_3)_2 \quad (\text{a})$ $\rightarrow \text{CH}_2=\text{C}=\text{CH}_2 + \text{CH}_2=\text{C}(\text{CH}_3)_2 \quad (\text{b})$							
1-Hexyne, 5-methyl-							
78 TSA3 ¹⁾ k _a . Bond-breaking reaction.	EX	990-1200	1.26(16)	0	36700±500	1	1.58
78 TSA3 ¹⁾ k _b . Molecular reaction.	EX	990-1200	2.00(12)	0	27500±1000	1	2.51
¹⁾ 5-Methyl-1-hexyne/Cyclohexene/Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexane. Similar data given in 76 TSA2. [5-Methyl-1-hexyne] = 0.02%. [Cyclohexene] = 0.01%. P(Ar) ~ (2-6) atm. [Toluene] = 1%.							
$\text{CH}_3\text{C}\equiv\text{CC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{C}=\text{C}(\text{CH}_3)_2 + \text{CH}_3$							
2-Pentyne, 4,4-dimethyl-							
81 KIN/NGU Thermolysis in a VLPP system. Mass-spectrometry.	EX	903-1246	2.51(16)	0	35934±755	1	2.0

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
<hr/>							
$\text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_2=\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$							
1,6-Heptadiene							
74 EGG/VIT3 Thermolysis in a static system.	EX	628-744	2.04(11)	0	23654±367	1	2.75
80 KIN VLP-Pyrolysis. RRKM extrapolation of VLFP data.	EX	794-1225	2.00(11)	0	23704±503	1	2.51
<hr/>							
$\text{cis-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$							
→ $\text{trans-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$ (a)							
→ $\text{CH}_2=\text{CHC}(\text{CH}_3)=\text{C}(\text{CH}_3)_2$ (b)							
1,3-Pentadiene, 2,3-dimethyl- (Z)-							
→ 1,3-Pentadiene, 2,3-dimethyl-, (E)- (a)							
→ 1,3-Pentadiene, 3,4-dimethyl- (b)							
71 FRE/LAM ¹⁾ k _a .	RN	473-517	1.78(12)	0	22096±192	1	1.35
71 FRE/LAM ¹⁾ k _b .	DE	473-517	9.33(10)	0	16732±108	1	1.26
¹⁾ Thermal isomerization in static system. Gas-chromatography. k is P-independent between 0.75 and 7.5 torr. k's determined from Equilibrium constants and the sums (k _a + k _{-a}) and (k _b + k _{-b}).							
<hr/>							
$\text{trans-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$							
→ $\text{cis-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$							
1,3-Pentadiene, 2,3-dimethyl-, (E)-							
→ 1,3-Pentadiene, 2,3-dimethyl-, (Z)-							
71 FRE/LAM Thermal isomerization in a static system. Gas-chromatography. k is P-independent between 0.75 and 7.5 torr. k determined from Equilibrium constant and the sum (k _f + k _r).	DE	473-517	2.29(12)	0	22770±192	1	1.35
<hr/>							
$\text{CH}_2=\text{CHC}(\text{CH}_3)=\text{C}(\text{CH}_3)_2 \rightarrow \text{cis-CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CHCH}_3$							
1,3-Pentadiene, 3,4-dimethyl-							
→ 1,3-Pentadiene, 2,3-dimethyl-, (Z)-							
71 FRE/LAM Thermal isomerization in a static system. Gas-chromatography. k is P-independent between 0.75 and 7.5 torr. k determined from Equilibrium constant and the sum (k _f + k _r).	DE	473-517	1.35(11)	0	17032±108	1	1.26

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
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Cyclohexene, 1-methyl-

78 SIM

EX 1000-1180 3.72(15) 0 35000 1

Single-pulse shock-tube.



→



(a)

→

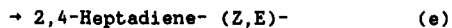
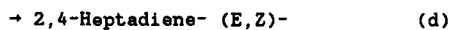
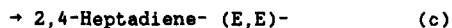
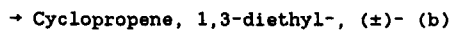
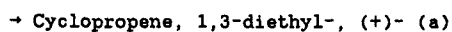


(b)

(racemic mixture)



Cyclopropene, 1,3-diethyl-, (-)-



73 YOR/DIT ¹⁾

EX 434-463 3.16(11) 0 16457±755 1 10.0

k_a .

Isomerization to the enantiomer.

73 YOR/DIT ¹⁾

EX 434-463 6.31(11) 0 16407±755 1 10.0

k_b .

Racemization.

(Loss of optical activity.)

73 YOR/DIT ¹⁾

EX 434-463 2.51(10) 0 16205±755 1 10.0

$k_c + k_d + k_e + k_f$, or $k_c + k_d + k_e$,

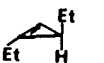

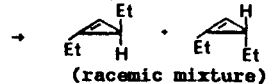
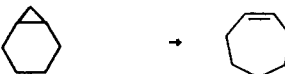
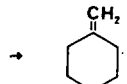
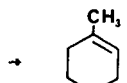
according to the mechanism proposed

in scheme V, or VI, respectively.

Isomerization by decyclization.

¹⁾ Static reactor pyrolysis.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 \rightarrow  (a)							
 (racemic mixture) (b)							
\rightarrow trans,trans- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CHCH}_2\text{CH}_3$ (c)							
\rightarrow trans,cis- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CHCH}_2\text{CH}_3$ (d)							
\rightarrow cis,trans- $\text{CH}_3\text{CH}=\text{CHCH}=\text{CHCH}_2\text{CH}_3$ (e)							
\rightarrow $\text{CH}_3\text{CH}_2\text{C}=\text{CCH}_2\text{CH}_2\text{CH}_3$ (f)							
Cyclopropene, 1,3-diethyl-, (+)-							
\rightarrow Cyclopropene, 1,3-diethyl-, (-)- (a)							
\rightarrow Cyclopropene, 1,3-diethyl-, (\pm)- (b)							
\rightarrow 2,4-Heptadiene- (E,E)- (c)							
\rightarrow 2,4-Heptadiene- (E,Z)- (d)							
\rightarrow 2,4-Heptadiene- (Z,E)- (e)							
\rightarrow 3-Heptyne (f)							
73 YOR/DIT ¹⁾ k_a . Isomerization to the enantiomer.	EX	434-463	3.16(11)	0	16457 \pm 755	1	10.0
73 YOR/DIT ¹⁾ k_b . Racemization.	EX	434-463	6.31(11)	0	16407 \pm 755	1	10.0
73 YOR/DIT ¹⁾ $k_c + k_d + k_e + k_f$, or $k_c + k_d + k_e$, according to the mechanism proposed in scheme V, or VI, respectively. Isomerization by decyclization.	EX	434-463	2.51(10)	0	16205 \pm 755	1	10.0
¹⁾ Static reactor pyrolysis.							
 (a)							
 (b)							
 (c)							
Bicyclo[4.1.0]heptane \rightarrow Cycloheptene (a)							
\rightarrow Cyclohexene, methylene- (b)							
\rightarrow Cyclohexene, 1-methyl- (c)							
73 FLO/PEN2 ¹⁾ k_a . Isomerization.	EX	708-769	6.61(14)	0	32662 \pm 503	1	1.91

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
73 FLO/PEN2 ¹⁾ k _b . Isomerization.	EX	708-769	1.20(15)	0	33166±705	1	2.69
73 FLO/PEN2 ¹⁾ k _c . Isomerization.	EX	708-769	9.5(14)	0	32511±856	1	3.16
¹⁾ Thermolysis in a static system. P ~ 4.5 torr.							
CH₃CH₂CH₂CH₂CH=CH₂ → products							
1-Heptene							
74 MAG/IOA	EX	823-923	3.55(13)	0	28334	1	
cis-CH₃CH₂CH₂CH=CHCH₃ → trans-CH₃CH₂CH₂CH=CHCH₃							
2-Heptene, (Z)-							
74 BAU/YAD	RL	1000-1150	1.0	0	0	1/1	
Rate-ratio assumed to be T-independent. k _{ref} : cis-CH ₃ CH=CHCH ₃ → trans-CH ₃ CH=CHCH ₃							
(CH₃)₂CHCH=C(CH₃)₂ → (CH₃)₂CCH=CHCH₃ + CH₃ (a) → (CH₃)₂C=CHCHCH₃ + CH₃ (b)							
2-Pentene, 2,4-dimethyl-							
73 TSA1	EX	1077-1151	~1.0(16)	0	35050	1	
1,1,2,2-Tetramethylcyclopropane/Cyclohexene/ Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexene. [Tetramethylcyclopropane] = 0.02%. [Cyclohexene] = 0.01%. [Toluene + Ar] = 1%.							
$\begin{array}{c} \text{CH}_3 \\ \\ \square \\ \\ \text{CH}_3 \end{array} \rightarrow \text{CH}_2=\text{CH}_2 + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2 \text{ (a)}$							
$\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2 \text{ (b)}$							
Cyclobutane, 1,1,2-trimethyl-							
→ Ethene + 2-Butene, 2-methyl- (a)							
→ 1-Propene + 1-Propene, 2-methyl- (b)							
71 COC/FRE3 ¹⁾ k _a .	EX	660-728	8.51(15)	0	32149±97	1	1.15
71 COC/FRE3 ¹⁾ k _b .	EX	660-728	5.62(15)	0	30282±116	1	1.17
¹⁾ Pyrolysis in a static system. k is P-independent within this P-range. P > 5 torr.							

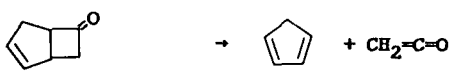

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\begin{array}{c} \text{H}_3\text{C} \diagdown \text{CH}_2 \\ \text{C} \diagup \text{CH}_2 \\ \text{H}_3\text{C} \diagup \end{array} \rightarrow (\text{CH}_3)_2\text{CCH}=\text{C}(\text{CH}_3)_2$						
Cyclopropane, 1,1,2,2-tetramethyl-						
→ 2-Pentene, 2,4-dimethyl-						
73 TSA1	EX	1077-1151	6.61(14)	0	31320	1
1,1,2,2-tetramethylcyclopropane/Cyclohexene/ Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexene. [Tetramethylcyclopropane] = 0.02%. [Toluene + Ar] = 1%. [Cyclohexene] = 0.01%.						
$(\text{CH}_3)_2\text{CCH}_2\text{C}(\text{CH}_3)_2 \uparrow \rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + (\text{CH}_3)_2\text{CH}$						
Butyl, 1,1,3-trimethyl-						
71 GEO/RAB	EX	298	2.11(7)			1
(CH ₃) ₂ CHCH ₂ C(CH ₃) ₂ † formed by: H + (CH ₃) ₂ CHCH ₂ C(CH ₃)=CH ₂						
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{CH}_3)_2 \uparrow \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3\text{CH}=\text{CH}_2$						
Butyl, 1,3,3-trimethyl-						
71 GEO/RAB	EX	298	1.70(8)			1
(CH ₃) ₃ CCH ₂ CHCH ₃ † formed by: H + (CH ₃) ₃ CCH ₂ CH=CH ₂						
$(\text{CH}_3)_2\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)_2\text{CH}_2 \rightarrow (\text{CH}_3)_2\text{CH} + (\text{CH}_3)_2\text{C}=\text{CH}_2 \quad (\text{a})$ $\rightarrow (\text{CH}_3)_2\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3 \quad (\text{b})$						
Butyl, 2,2,3-trimethyl-						
81 BAL/WAL2 1) 3)	ES	753	(2.4±0.6)(6)			1
81 BAL/WAL2 1) 3) 1) k _a .	EX	298-753	6.31(13)	0	12870±842	1 3.16
81 BAL/WAL2 2) 3)	RN	753	(2.4±0.6)(5)			1
81 BAL/WAL2 2) 3) 2) k _b .	RN	298-753	6.3(13)	0	14554±842	1 3.16
3) Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric-acid-coated reaction vessels. Estimations based on a proposed mechanism. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.						
$(\text{CH}_3)_3\text{CCH}(\text{CH}_3)\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_3\text{CH}=\text{CH}_2 \quad (\text{a})$ $\rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}_2 + \text{CH}_3 \quad (\text{b})$						
Butyl, 2,3,3-trimethyl-						
81 BAL/WAL2 1) 3)	ES	753	1.3(6)			1

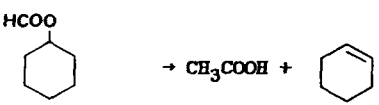
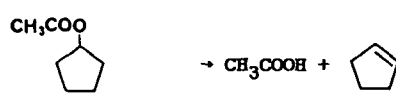
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
81 BAL/WAL2 1) 3) 1) k_a .	ES	298-753	6.31(13)	0	13352±842	1	3.16
81 BAL/WAL2 2) 3)	RN	753	(6.2±3.1)(4)			1	
81 BAL/WAL2 2) 3) 2) k_b . 3) Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric-acid-coated reaction vessels. Estimations based on a proposed mechanism. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.	RN	298-753	6.31(13)	0	15637±842	1	3.16
$(CH_3)_3CC(CH_3)_2 \rightarrow (CH_3)_2C=CH_2 + (CH_3)_2CH$ (a) $\rightarrow (CH_3)_2C=C(CH_3)_2 + CH_3$ (b)							
Propyl, 1,1,2,2-tetramethyl-							
81 BAL/WAL2 1) 2)	RN	753	(7.4±2.5)(5)			1	
81 BAL/WAL2 1) 2) 1) k_a . 2) Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric-acid-coated reaction vessels. Estimations based on a proposed mechanism. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.	RN	298-753	6.31(13)	0	13712±842	1	3.16
80 BAL/WAL k_b . Decomposition of 2,2,3-Trimethylbutane in presence of O ₂ . P = (60-500) torr.	RN	953	1.4(3)			1	
$(CH_3)_3CC(CH_3)_2 + O_2 \rightarrow (CH_3)_3CC(CH_3)=CH_2 + HO_2$							
Propyl, 1,1,2,2-tetramethyl- + Oxygen molecule							
80 BAL/WAL k_{ref} : $(CH_3)_3CC(CH_3)_2 \rightarrow (CH_3)_2C=C(CH_3)_2 + CH_3$ Decomposition of 2,2,3-Trimethylbutane in presence of O ₂ . P = (60-500) torr.	RL	773	(9.4±1.8)(7)			2/1	
81 BAL/WAL2 1) k_{ref} : $(CH_3)_3CC(CH_3)_2 \rightarrow (CH_3)_2C=CH_2 + (CH_3)_2CH$	RL	753	(1.75±0.20)(5)			2/1	
81 BAL/WAL2 1) 1) Oxidation of 2,2,3-Trimethylbutane in H ₂ /O ₂ mixtures, in aged boric-acid-coated reaction vessels. Estimation based on a proposed mechanism. P(Total) = 500 torr. P(2,2,3-Trimethylbutane) = 5 torr.	RN	753	(1.3±0.2)(11)			2	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
CH₃(CH₂)₅CH₃ → products						
Heptane						
73 ILL/WEL	EX	873-1073	(1.89±0.03)(12)	0	26447	1
75 TAN/KRA	EX	763-813	1.58(10)	0	24660	1
75 TAN/KRA	EX	763-813	1.6(10)	0	24660	1
Thermolysis in a static reactor.						
P = (75-150) torr.						
79 BAJ/VES	EX	953-1033	1.3(11)	0	23516	1
Thermolysis in a tubular flow-reactor.						
P ~ 1 atm.						
(CH₃)₂CHCH₂CH(CH₃)₂ → products						
Pentane, 2,4-dimethyl-						
73 ILL/WEL	EX	873-1073	(4.48±0.12)(14)	0	31228	1
(CH₃)₃CCH(CH₃)₂ → (CH₃)₃C + (CH₃)₂CH						
Butane, 2,2,3-trimethyl-						
80 BAL/WAL	EX	953-1198	2.88(16)	0	36687±180	1 1.32
Decomposition of 2,2,3-Trimethylbutane						
in presence of O ₂ .						
P = (60-500) torr.						
						
Bicyclo[3.2.0]hept-2-en-6-one						
→ 1,3-Cyclopentadiene + Ethenone						
72 EGG/COC	EX	471-534	1.45(13)	0	18888±126	1 1.29
Pyrolysis in a static system.						
P ₀ = (15-485) torr.						
						
Bicyclo[3.2.0]heptan-6-one → Cyclopentene + Ethenone						
72 COC/EGG4	EX	546-652	1.62(14)	0	24434±146	1 1.26
Pyrolysis in a static system.						
P ₀ = (3.8-40) torr.						
CH₂=C=CHC(CH₃)₂COOH → CH₂=CHCH=C(CH₃)₂ + CO₂						
3,4-Pentadienoic acid, 2,2-dimethyl-						
76 BIG/WEA2	EX	500	2.16(-6)			1
76 BIG/WEA2	EX	630	6.49(-3)			1
76 BIG/WEA2	EX	500-695	1.67(11)	0	19455±758	1 2.6
A and B recalculated from the reported data.						

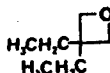
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}(\text{CH}_3)_2 + \text{CO}_2$							
3-Butenoic acid, 2,2,3-trimethyl-							
82 ALB/BIG ¹⁾	EX	577	1.2(-2)				1
82 ALB/BIG ¹⁾	EX	~577	1.04(11)	0	17176		1
A and B recalculated from the reported data.							
1) Pyrolysis in a flow-reactor.							
NMR-spectrometry.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$							
4-Penten-1-ol acetate							
79 MAR/HER	EX	513-693	6.46(12)	0	24538±541	1	2.29
Pyrolysis in a static system.							
P = (44-282) torr.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}=\text{CH}_2$							
→ $\text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{CH}=\text{CH}_2$ (a)							
→ $\text{CH}_3\text{COOH} + \text{CH}_3\text{CH}=\text{CHCH}=\text{CH}_2$ (b)							
4-Penten-2-ol acetate							
79 MAR/HER	EX	513-693	2.19(12)	0	21435±349	1	1.78
$k_a + k_b$.							
Pyrolysis in a static system.							
P = (44-282) torr.							
$\text{trans-CH}_3\text{CH}=\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2$							
→ $\text{trans-CH}_3\text{CH}=\text{CHCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
2-Butenoic acid, (E)-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(7.10±0.20)(-3)				1
							
Formic acid cyclohexyl ester (Cyclohexyl formate)							
→ Formic acid + Cyclohexene							
72 TIN/KOO	EX	623-673	1.26(12)	0	21641±1007	1	3.98
Thermolysis.							
							
Cyclopentanol acetate → Acetic acid + Cyclopentene							
72 TIN/KOO	EX	588-663	1.58(12)	0	20835±503	1	3.98
Thermolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\begin{array}{c} \text{CH}_3 \\ \triangle \\ \\ \text{C}-\text{COOH} \\ \\ \text{CH}_3 \end{array} \rightarrow \text{CH}_3\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2 \text{ (a) = (b)}$ $\rightarrow (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)_2 + \text{CO}_2 \text{ (c)}$						
Cyclopropaneacetic acid, α, α -dimethyl-						
→ 2-Pentene, 2-methyl- + Carbon dioxide (a) = (b)						
→ 2-Butene, 2,3-dimethyl- + Carbon dioxide (c)						
79 BIG/FET 2)	EX	725	1.31(-3)			1
$k_a = k_b$.						
79 BIG/FET 2)	EX	725	<5.0(-5)			1
k_c . Upper-limit k.						
79 BIG/FET 1) 2)	EX	725	2.62(-3)			1
79 BIG/FET 1) 2)	EX	690-740	(1.74±0.07)(11)	0	23074±348	1
A and B recalculated from the reported data.						
1) $k_a + k_b + k_c$.						
2) Pyrolysis in a Flow-reactor with evacuated sealed tubes.						
Gas-chromatography. NMR-spectroscopy.						
$\begin{array}{c} \text{H}_3\text{C} \\ \triangle \\ \\ \text{H}_3\text{C}-\text{C}-\text{CH}_2\text{COOH} \\ \\ \text{H}_3\text{C} \end{array} \rightarrow (\text{CH}_3)_3\text{CCH}=\text{CH}_2 + \text{CO}_2 \text{ (a)}$ $\rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{CH}=\text{CH}_2 + \text{CO}_2 \text{ (b)}$ $\rightarrow (\text{CH}_3)_2\text{CHC}(\text{CH}_3)=\text{CH}_2 + \text{CO}_2 \text{ (c)}$						
Cyclopropaneacetic acid, 2,2-dimethyl-						
→ 1-Butene, 3,3-dimethyl- + Carbon dioxide (a)						
→ 1-Pentene, 4-methyl- + Carbon dioxide (b)						
→ 1-Butene, 2,3-dimethyl- + Carbon dioxide (c)						
80 BIG/FET 2)	EX	725	8.2(-4)			1
k_a .						
80 BIG/FET 2)	EX	725	4.8(-4)			1
k_b .						
80 BIG/FET 2)	EX	725	1.0(-4)			1
k_c .						
80 BIG/FET 1) 2)	EX	725	1.4(-3)			1
80 BIG/FET 1) 2)	EX	750-820	4.49(11)	0	24215±722	1
A and B recalculated from the reported data.						
1) $k_a + k_b + k_c$.						
2) Pyrolysis in a flow-reactor with evacuated sealed tubes.						
Gas-chromatography. NMR-spectrometry.						
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{CH}_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{C}(\text{O})\text{CH}_3$						
2-Pentanone, 5-acetyloxy-						
76 DEB/TAY	EX	650-700	6.31(12)	0	23905	1

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A units	k err. factor
CH₃C(O)OC(CH₃)₂C(O)CH₃ → CH₃COOH + CH₂=C(CH₃)C(O)CH₃							
2-Butanone, 3-(acetyloxy)-3-methyl-							
76 CHU/MAR ¹⁾	EX	573	9.54(-4)			1	
76 CHU/MAR ¹⁾	EX	543-593	2.88(13)	0	21741±201	1	1.48
¹⁾ Thermolysis in a clean or seasoned Pyrex vessel.							
P = (69-222) torr.							
CH₃C(O)OC(CH₃)₂C(O)OCH₃ → CH₃COOH + CH₂=C(CH₃)C(O)OCH₃							
Propanoic acid, 2-(acetyloxy)-2-methyl-, methyl ester							
80 MAR/CHU	EX	503-613	3.39(12)	0	21182±433	1	2.09
Pyrolysis in a static system. Mass-spectrometry.							
IR-, and NMR-spectroscopy.							
P = (56-210) torr.							
							
→ HCCHO + (CH ₃ CH ₂) ₂ C=CH ₂							
Oxetane, 3,3-diethyl-							
→ Formaldehyde + Pentane, 3-methylene-							
75 CLE/FRE	EX	675-736	1.98(15)	0	30053±101	1	1.16
Thermolysis in a static system.							
CH₃C(O)OCH₂CH₂CH(CH₃)₂ → CH₃COOH + CH₂=CHCH(CH₃)₂							
1-Butanol, 3-methyl-, acetate							
79 CHU/MAR	EX	633-693	5.37(12)	0	24358±457	1	1.95
Pyrolysis in a static system.							
P = (63-250) torr.							
79 TAY	EX	660-712	6.61(12)	0	24509	1	
Pyrolysis in a stainless-steel reactor.							
CH₃C(O)OCH₂CH₂CH(CH₃)₂ + O₂(¹A_g) → products							
1-Butanol, 3-methyl-, acetate + Oxygen molecule							
79 DAT/RAO	EX	298	(5.2±1.1)(6)			2	
Microwave discharge flow system.							
CH₃C(O)OC(CH₃)₂CH₂CH₃ → CH₃COOH + (CH₃)₂C=CHCH₃ (a)							
→ CH₃COOH + CH₃CH₂C(CH₃)=CH₂ (b)							
2-Butanol, 2-methyl-, acetate							
72 TIN/KOO	EX	535-596	1.58(12)	0	19376±503	1	2.51
k _a . Thermolysis.							
72 TIN/KOO	EX	535-596	5.01(12)	0	19376±503	1	2.51
k _b . Thermolysis.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}(\text{CH}_3)_2$							
$\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}(\text{CH}_3)_2$ (a)							
$\rightarrow \text{CH}_3\text{COOH} + \text{CH}_3\text{CH}=\text{C}(\text{CH}_3)_2$ (b)							
2-Butanol, 3-methyl-, acetate							
73 CHU/MAR	EX	583-643	1.33(13)	0	22934±242	1	1.01
$k_a + k_b$.							
Pyrolysis in a static system.							
Channel (a) is predominant.							
P = (30-300) torr.							
$(\text{CH}_3)_2\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Propanoic acid, 2-methyl-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.80±0.20)(-3)			1	
$\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{CH}_2\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$							
Propanoic acid 1,1-dimethylethyl ester							
78 TAY	EX	543-620	3.63(12)	0	19341	1	
Pyrolysis in a stainless-steel reactor.							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Butanoic acid 1-methylethyl ester							
77 SMI/MUT	EX	651	(5.93±0.27)(-3)			1	
78 CHU/MAR ¹⁾	EX	603	4.07(-4)			1	
78 CHU/MAR ¹⁾	EX	583-622	2.45(13)	0	23301±252	1	1.58
¹⁾ Pyrolysis in a static system.							
$\text{CH}_3\text{CH}_2\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_3$							
$\rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$							
Carbonic acid dipropyl ester (Di-n-propyl carbonate)							
72 BIG/WRE1 ¹⁾	EX	700	(7.35±0.22)(-2)			1	
72 BIG/WRE1 ¹⁾	EX	663-708	(4.02±0.12)(13)	0	23754	1	
The A-factor recalculated from the reported experimental data.							
¹⁾ Pyrolysis in the Kooyman flow-tube.							
72 BIG/WRE3	EX	629	1.42(-3)			1	
Flow-tube method.							
76 CRO/HUN	EX	583-667	9.33(11)	0	21892	1	
$(\text{CH}_3)_2\text{CHOC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3\text{CH}=\text{CH}_2 + \text{CO}_2 + (\text{CH}_3)_2\text{CHOH}$							
Carbonic acid bis(1-methylethyl) ester (Di-i-propyl carbonate)							
72 BIG/WRE2 ¹⁾	EX	629	3.99(-2)			1	


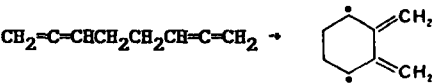
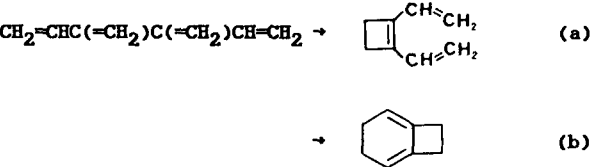
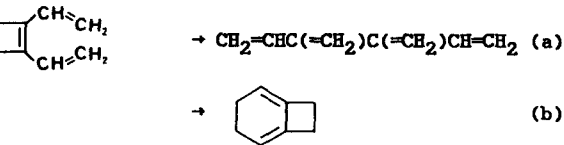
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 BIG/WRE2 ¹⁾ The A-factor recalculated from the reported data. ¹⁾ Flow-tube pyrolysis.	EX	593-648	2.20(14)	0	22798	1
$(\text{CD}_3)_2\text{CHOC}(\text{O})\text{CH}(\text{CD}_3)_2 \rightarrow \text{CD}_3\text{CH}=\text{CD}_2 + \text{CO}_2 + (\text{CD}_3)_2\text{CHOD}$						
Carbonic acid bis(1-methyl-d ₃ -ethyl-2,2,2-d ₃) ester						
72 BIG/WRE2 ¹⁾	EX	629	1.66(-2)			1
72 BIG/WRE2 ¹⁾ The A-factor recalculated from the reported data. ¹⁾ Flow-tube pyrolysis.	EX	593-648	2.39(14)	0	23402	1
$\text{CH}_3\text{OCH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{OCH}_2\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$						
Acetic acid, methoxy-, 1,1-dimethylethyl ester						
78 TAY Pyrolysis in a stainless-steel reactor. Gas-chromatography.	EX	528-587	3.09(13)	0	20232	1
$\text{CH}_3\text{OC}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}_3$						
→ $\text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (a)						
→ $\text{CH}_3\text{OH} + \text{CO}_2 + (\text{CH}_3)_2\text{C}=\text{CHCH}_3$ (b)						
Carbonic acid 1,1-dimethylpropyl methyl ester						
72 BIG/WRE3	EX	629	3.48			1
72 BIG/WRE3 $k_a + k_b$. Flow-tube method. Assumed T-range, omitted in text. The A-factor recalculated from the reported data.	EX	593-648	3.97(12)	0	17464	1
$\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OOH} \rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{O} + \text{OH}$						
Hydroperoxide, heptyl- → Heptoxy + Hydroxyl						
80 SAH/HEI Decomposition in a Pyrex reactor with continuous flow. Gas-chromatography. P = 100 torr.	EX	540-625	≈3.0(15)	0	21750±500	1
82 SAH/HEI1 Decomposition in a flow system, in a mixture containing O ₂ , H ₂ and CO ₂ . Thin-layer and liquid-phase Gas-chromatography. [Hydroperoxide] = 1.23x10 ¹⁸ molec.cm ⁻³ . P = 100 torr.	EX	523-633	(1.10±0.25)(16)	0	21892±503	1

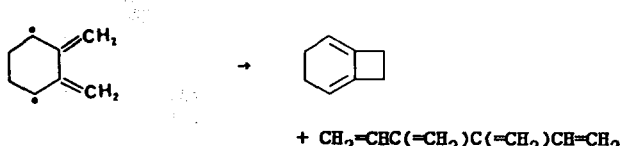
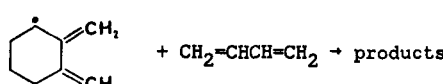
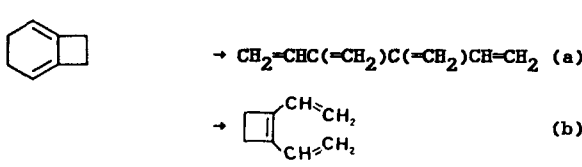
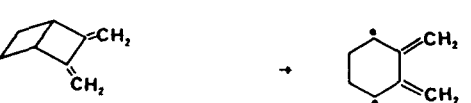
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3(\text{CH}_2)_4\text{CH}(\text{OOH})\text{CH}_3 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{CH}(\text{O}^\cdot)\text{CH}_3 + \text{OH}$						
Hydroperoxide, 1-methylhexyl-						
82 SAN/HEI1 Decomposition in a flow system, in a $\text{O}_2/\text{H}_2/\text{CO}_2$ mixture. Thin-layer and liquid-phase Gas-chromatography. [Hydroperoxide] = 1.23×10^{18} molec. cm^{-3} . P = 100 torr.	EX	523-633	(7.0±2.0)(15)	0	20886±503	1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{SCH}_2\text{CH}=\text{CH}_2 \rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{S} + \text{CH}_3\text{CH}=\text{CH}_2$						
Butane, 1-(2-propenylthio)- → Butanethial + 1-Propene						
82 MAR/DRA Pyrolysis in a static system. Gas-chromatography. NMR-, and Mass-spectrometry. Butanethial trimerizes to the cyclic compound 2,4,6-Tripropyl-1,3,5-trithiane. $P_0 = (87-685)$ torr.	EX	535-566	2.63(11)	0	18644±361	1 1.91
$(\text{CH}_3)_3\text{CN}=\text{NCH}_2\text{CH}=\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{C} + \text{CH}_2\text{CH}=\text{CH}_2 + \text{N}_2$						
Diazene, (1,1-dimethylethyl)-2-propenyl-						
72 CRA/TAK Thermolysis. Mass-spectrometry. Gas-chromatography. In presence of ^{15}NO . P(Total) = (50-60) torr.	EX	354-399	5.37(12)	0	14997±151	1 1.82
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_2\text{NH} + \text{CO}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$						
Carbamic acid, dimethyl-, 1,1-dimethylethyl ester						
72 DAL/ZIO2 Thermolysis in a conventional static system.	EX	323-333	7.41(12)	0	18993±201	1
72 KWA/SLU Thermolysis in a conventional static system.	EX	575-636	1.86(13)	0	19628±50	1 1.07
$(\text{CH}_3)_2\text{NC}(\text{O})\text{OC}(\text{CD}_3)_3 \rightarrow (\text{CH}_3)_2\text{ND} + \text{CO}_2 + (\text{CD}_3)_2\text{C}=\text{CD}_2$						
Carbamic acid, dimethyl-, (1,1-dimethyl- d_9) ester						
72 KWA/SLU Thermolysis in a conventional static system.	EX	584-647	2.34(13)	0	20282±50	1 1.12

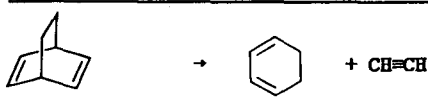
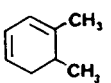
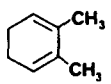
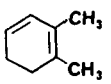
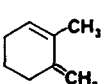
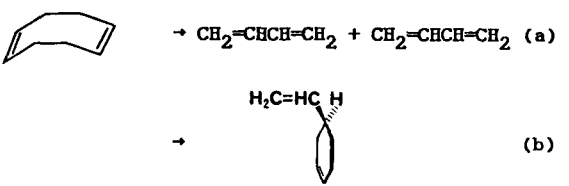
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 <p>1,3-Cyclohexadiene, 5,6-bis(methylene)- → Bicyclo[4.2.0]octa-1,3,5-triene</p>	EX	594-757	(2.1±1.1)(12)	0	13538±352	1
81 ROT/SCH Thermal isomerization behind incident shock-waves in N ₂ , or He as carrier gas. UV-spectrometry.						
 <p>1,2,6,7-Octatetraene → 1,4-Cyclohexadiene, 2,3-bis(methylene)-</p>	EX	369-455	(6.1±0.8)(9)	0	12380±50	1
82 ROT/SCH2 Thermal rearrangement in an air thermostat. P = (5.3-585) torr.						
 <p>1,5-Hexadiene, 3,4-bis(methylene)- → Cyclobutene, 1,2-diethenyl- (a) → Bicyclo[4.2.0]octa-1,5-diene (b)</p>	EX	495-549	(2.5±1.3)(11)	0	17967±252	1
82 ROT/SCH2 ¹⁾ k _a .						
82 ROT/SCH2 ¹⁾ k _b .	EX	495-549	(2.4±1.0)(10)	0	16960±201	1
1) Thermal rearrangement in an air thermostat. P = (5.3-585) torr.						
 <p>Cyclobutene, 1,2-diethenyl- → 1,4-Hexadiene, 3,4-bis(methylene)- (a) → Bicyclo[4.2.0]octa-1,5-diene (b)</p>	EX	424-479	(4.8±0.7)(13)	0	17967±50	1
82 ROT/SCH2 k _a .						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
82 ROT/SCH2 k_b . Thermal rearrangement in an air thermostat. P = 5.3-585) torr.	EX	424-479	(3.0±0.8)(11)	0	14947±101	1
 <p>1,4-Cyclohexanediyl, 2,3-bis(methylene)- → Bicyclo[4.2.0]octa-1,5-diene + 1,5-Hexadiene, 3,4-bis(methylene)-</p>						
82 ROT/SCH1 Thermal rearrangement in an air thermostat.	RL	318-356	(7.4±8.9)(2)	0	5788±403	1/2
k_{ref} :  <p>+ CH₂=CHCH=CH₂ → products</p>						
 <p>Bicyclo[4.2.0]octa-1,5-diene → 1,5-Hexadiene, 3,4-bis(methylene)- (a) → Cyclobutene, 1,2-diethenyl- (b)</p>						
82 ROT/SCH2 ¹⁾ k_a .	EX	486-518	(2.4±1.3)(14)	0	21087±252	1
82 ROT/SCH2 ¹⁾ k_b .	EX	495-549	(1.6±0.3)(13)	0	19124±50	1
¹⁾ Thermal rearrangement in an air thermostat. P = (5.3-585) torr.						
 <p>Bicyclo[2.2.0]hexane, 2,3-bis(methylene)- → 1,4-Cyclohexanediyl, 2,3-bis(methylene)-</p>						
82 ROT/SCH1 Thermal rearrangement in an air thermostat.	EX	318-368	(8.8±2.1)(12)	0	12984±101	1

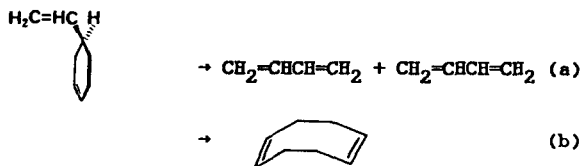
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 <p>Bicyclo[2.2.2]octa-2,5-diene → 1,3-Cyclohexadiene + Ethyne</p>	EX	354-435	1.14(14)	0	16366±20	1	1.05
<p>82 HUY/LEE Thermolysis. Static system. P = (0.5-6.0) torr.</p>							
<p>trans,trans,trans-CH₃CH=CHCH=CHCH=CH₃</p> <p>→  (a)</p> <p>→  (b)</p> <p>→  (c)</p> <p>→  (d)</p> <p>→ any other products (e)</p>							
<p>2,4,6-Octatriene, (E,E,E)-</p> <p>→ 1,3-Cyclohexadiene, 1-6-dimethyl- (a)</p> <p>→ 1,3-Cyclohexadiene, 2,3-dimethyl- (b)</p> <p>→ 1,3-Cyclohexadiene, 1,2-dimethyl- (c)</p> <p>→ Cyclohexene, 1-methyl-6-methylene- (d)</p> <p>→ other products (e)</p>	EX	533-583	2.89(13)	0	22748±327	1	1.78
<p>73 DOE/BEA k_{overall}. Thermal isomerization.</p> <p></p>							
<p>1,5-Cyclooctadiene, (Z,Z)-</p> <p>→ 1,3-Butadiene (a)</p> <p>→ Cyclohexene, 4-ethenyl- (b)</p>	EX	575-630	2.00(16)	0	28148±468	1	1.86
<p>72 DOE/FRA¹) k_a. Thermal dissociation.</p>							

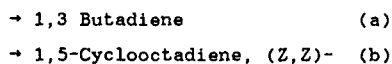
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
77 HUY/LUY ²⁾ k _a . Thermal dissociation.	EX	505-586	2.88(16)	0	28374±50	1	1.10
72 DOE/FRA ¹⁾ k _b . Thermal rearrangement.	EX	575-630	3.55(15)	0	26371±574	1	2.19
77 HUY/LUY ²⁾ k _b . Thermal rearrangement.	EX	505-586	2.19(15)	0	26059±60	1	1.12
72 DOE/FRA ¹⁾ k _a + k _b . Overall reaction.	EX	575-630	9.77(15)	0	26819±382	1	1.70

1) Pyrolysis in a 3.5 l. lead-potash glass vessel.
2) Thermal reaction. Static system.
P = (15-51) torr.

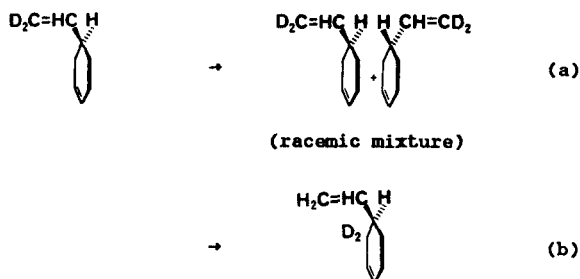


Cyclohexene, 4-ethenyl-

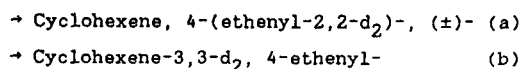


77 HUY/LUY ¹⁾ k _a . (k _a = k _{-a} K.)	DE	464-557	2.51(14)	0	30297±252	1	3.16
77 HUY/LUY ¹⁾ k _b . (k _b = k _{-b} K.)	DE	464-557	7.94(13)	0	29995±352	1	3.16

1) Thermal reaction of 1,3-Butadiene and 1,5-Cyclooctadiene. Static system.






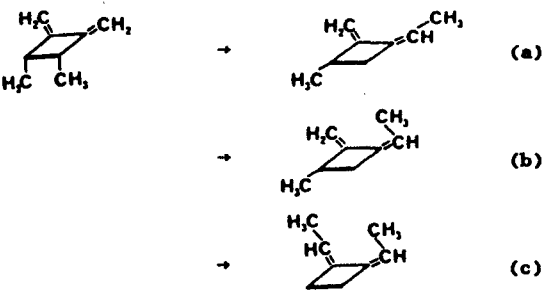
Cyclohexene, 4-(ethenyl-2,2-d₂)-, (R)-



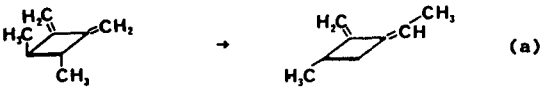
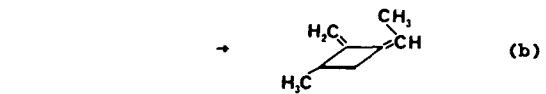
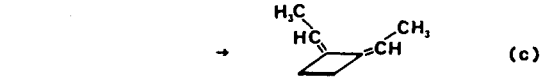
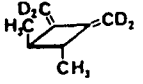
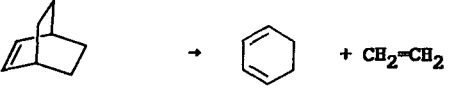
72 DOE/FRA ¹⁾ k _a . Thermal racemization.	EX	575-630	1.23(12)	0	24987±400	1	1.82
72 DOE/FRA ¹⁾ k _b . Thermal rearrangement.	EX	575-630	1.23(13)	0	26241±896	1	4.17

1) Pyrolysis in a 12 liter Pyrex vessel.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 <p>1,4-Cyclohexadiene, 1-ethyl- → Benzene, ethyl- + Hydrogen molecule</p> <p>72 COC/FRE Pyrolysis in a static system. P₀ = 10 torr.</p>	EX	589-652	1.32(13)	0	23085±126	1	1.23
 <p>1,4-Cyclohexadiene, 1,2-dimethyl- → Benzene, 1,2-dimethyl- (o-Xylene) + Hydrogen molecule</p> <p>72 COC/FRE Pyrolysis in a static system. P₀ = (3-4) torr.</p>	EX	572-627	3.47(12)	0	22003±40	1	1.07
 <p>Cyclobutane, 1,2-diethenyl-, trans- → products</p> <p>81 GRI/SCH Thermal rearrangement in an air thermostat. P = (2-3) torr.</p>	EX	448-503	(1.93±0.31)(13)	0	17861±75	1	
 <p>Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, cis- → Cyclobutane, 1-ethylidene-3-methyl- 2-methylene-, (E)- (a) → Cyclobutane, 1-ethylidene-3-methyl- 2-methylene-, (Z)- (b) → Cyclobutane, 1,2-diethylidene-, (E,Z)- (c)</p> <p>82 GAJ/BEN k_a + k_b + k_c. Thermal isomerization in a flow-reactor. Channel (b) predominant.</p>	EX	588-648	5.01(13)	0	21238	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k _A	k _{err.}
  							
Cyclobutane, 1,2-dimethyl-3,4-bis(methylene)-, trans-							
→ Cyclobutane, 1-ethylidene-3-methyl-2-methylene-, (E)- (a)							
→ Cyclobutane, 1-ethylidene-3-methyl-2-methylene-, (Z)- (b)							
→ Cyclobutane, 1,2-diethylidene-, (E,E)- (c)							
82 GAJ/BEN 1) 2)	EX	588-648	3.98(13)	0	21087	1	
82 GAJ/BEN 1) 2)	EX	503	2.31(-5)			1	
1) $k_a + k_b + k_c$.							
82 GAJ/BEN 2)	EX	503	(1.08±0.01)			1/1	
$(k_a + k_b + k_c)/k_{ref}$.							
k_{ref} :  → products.							
(Isotope effect)							
2) Thermal isomerization in a flow-reactor.							
Step (a) predominant.							
							
Bicyclo[2.2.2]oct-2-ene → 1,3-Cyclohexadiene + Ethene							
71 COC/FRE1	EX	649-718	2.88(15)	0	29398±81	1	1.12
Retrodiene thermolysis in a static system.							
Gas. chromatography. P-independent above 4 torr.							
80 HUY/RIG	EX	548-632	1.32(15)	0	28837±50	1	1.10
Retro-Diels-Alder pyrolysis of							
Bicyclo[2.2.2]oct-2-ene in a static system.							
Gas-chromatography.							
$CH_3C=CCH_2CH_2CH(CH_3)_2 \rightarrow CH_3C=CCH_2 + CH_2CH(CH_3)_2$ (a)							
$\rightarrow CH_3CH=C=CH_2 + CH_2=C(CH_3)_2$ (b)							
2-Heptyne, 6-methyl-							
78 TSA3 1)	EX	990-1200	1.58(16)	0	36800±500	1	1.61
k_a . Bond-breaking reaction.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
78 TSA3 ¹⁾ k _b . Molecular reaction.	EX	990-1200	2.00(12)	0	28700±1000	1	2.51
¹⁾ 6-Methyl-2-heptyne/Cyclohexene/Toluene/Ar thermolysis in a single-pulse shock-tube. k's determined relative to the decomposition of Cyclohexene. Similar data given in 76 TSA2. [Cyclohexene] = 0.01%. [Toluene] = 1%. [6-Methyl-2-heptyne] = 0.02%. P(Ar) ~ (2-6) atm.							
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ → $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$ (a) → $\text{CH}_3\text{CH}_2\text{CHCH}_3 + \text{CH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (b)							
1-Hexene, 2,4-dimethyl-							
73 TSA2 ¹⁾ ²⁾	EX	996-1180	2.82(12)	0	26900±250	1	1.38
78 TSA5 ¹⁾ ²⁾	EX	996-1180	3.16(12)	0	26900	1	
¹⁾ k _a . 1050 K given by the author as central-T.							
73 TSA2 ²⁾	EX	1050	4.27(15)	0	33200±150	1	1.17
k _b .							
²⁾ Single-pulse shock-tube.							
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)_2\text{CH}_2 \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_2=\text{CH}_2$ (a) → $(\text{CH}_3)_3\text{CC}(\text{CH}_3)=\text{CH}_2 + \text{CH}_3$ (b)							
Butyl, 2,2,3,3-tetramethyl-							
79 BAL/WAL2 ¹⁾	RL	753	5.77(-3)				1/1
k _b /k _a .							
79 BAL/WAL2 ¹⁾	RN	753	1.88(6)				1
k _a .							
79 BAL/WAL2 ¹⁾	RN	753	1.08(4)				1
k _b .							
¹⁾ Oxidation in aged boric-acid-coated vessels. Gas-chromatography. Absolute k's determined on the basis of Benson's additivity rules.							
$\text{CH}_3(\text{CH}_2)_6\text{CH}_3 \rightarrow \text{products}$							
Octane							
73 ILL/WEL	EX	873-1073	(1.04±0.02)(12)	0	26336	1	
80 RUM/SHE	EX	893-993	4.07(13)	0	29867±1516	1	4.90
Pyrolysis in a quartz reactor. P = 760 torr.							
$(\text{CH}_3)_2\text{CH}(\text{CH}_2)_4\text{CH}_3 \rightarrow \text{products}$							
Heptane, 2-methyl-							
73 ILL/WEL	EX	873-1046	(1.52±0.04)(13)	0	28143	1	



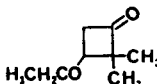
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_3)_3\text{CC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_3\text{C} \quad (\text{a})$ $\rightarrow (\text{CH}_3)_2\text{C}=\text{CH}_2 + (\text{CH}_3)_3\text{CH} \quad (\text{b})$							
Butane, 2,2,3,3-tetramethyl- (Hexamethylethane)							
74 GOL/ALF k_a . Best fit of experimental data to $\log A = 16.4$ for each C-C fission.	DE	850-1150	2.51(16)	0	34222	1	
78 ATR/BAL ¹⁾ k_a .	EX	985	2.37(1)			1	
78 ATR/BAL ¹⁾ k_a .	EX	1141	2.75(3)			1	
78 ATR/BAL ¹⁾ k_a . Based on the above data combined with those from 78 TSA4.	SE	713-813	6.03(16)	0	34931±180	1	1.36
¹⁾ Oxidation in KCl-coated vessels. P = (60-500) torr.							
78 TSA4 ²⁾ k_a .	EX	990-1100	2.51(16)	0	34400	1	
78 TSA4 ²⁾ k_a . Extrapolation over the given T-range.	EX	300-1100	2.00(17)	0	36600	1	
²⁾ Single-pulse shock-tube.							
79 WAL/TSA k_a . Thermolysis of 6-Methyl-2-heptyne in a flow-system, in He, in presence of 1-Methyl-cyclohexene and Toluene. k 's determined relative to the decomposition of 1-Methylcyclohexene. [1-Methylcyclohexene] = (0.08-0.12)%. [Hexamethylethane] = (0.003-0.04)%. [Toluene] = (2.0-13.6)%.	EX	700-900	2.51(17)	0	36300±200	1	1.58
82 BAL/HIS k_a . Decomposition of Hexamethylethane in KCl-coated-, or Pyrex-aged-boric- acid-coated vessels. Gas-chromatography. P = (1.0-4.0) torr.	EX	673-815	1.04(17)	0	35448±361	1	
78 BAL/EVA k_p . Decomposition in cylindrical KCl-coated Pyrex vessels. P = (60-500) torr.	EX	693-813	7.76(13)	0	33078±168	1	1.26
78 TAY/MIL k_{total} . Pyrolysis in wal-less reactor. The products are: 2-Methylpropene, Hydrogen, 1-Propene, 2-Methyl-2-butene, Ethane, Methane, Neopentane and 2,3-Dimethyl-2-butene, in order of abundance.	EX	750-950	5.01(10)	0	21741	1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A units	k err. factor
 \rightarrow products							
Bicyclo[3.2.0]hept-3-en-6-one, 5-methyl- 72 COC/EGG3 Pyrolysis in a static system. Gas-chromatography. P = (2.7-20) torr.	EX	489-565	3.16(14)	0	22108±337	1	1.91
$\text{CH}_2\text{CH}=\text{CH}_2\text{OC}(\text{O})\text{C}(\text{O})\text{OCH}_2\text{CH}=\text{CH}_2 \rightarrow 2\text{CO}_2 + 2\text{CH}_2=\text{CHCH}_2$ Ethanedioic acid di-2-propenyl ester 76 SAK/NOH Pyrolysis in a flow-reactor.	EX	723-763	7.94(10)	0	21741	1	
80 NOH/SAK ¹⁾	EX	703-783	2.00(10)	0	22610	1	
81 NOH/SAK ¹⁾	EX	723-783	6.31(10)	0	21651	1	
¹⁾ Pyrolysis in a flow-reactor. Gas-chromatography. Mass-spectrometry.							
$\text{CH}_2=\text{CHCH}=\text{CHC}(\text{CH}_3)_2\text{COOH} \rightarrow \text{CH}_2=\text{CHCH}_2\text{CH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ 3,5-Hexanedioic acid, 2,2-dimethyl- 76 BIG/WEA2 76 BIG/WEA2 76 BIG/WEA2 A and B recalculated from the reported data.	EX	500	7.35(-8)			1	
	EX	692	2.90(-2)			1	
	EX	500-723	1.42(13)	0	23389±758	1	
$\text{CH}_2=\text{CHCH}=\text{CHC}(\text{CH}_3)_2\text{COOD} \rightarrow \text{CH}_2=\text{CHCHDCH}=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ 3,5-Hexanedioic acid-d, 2,2-dimethyl- 76 BIG/WEA2	EX	692	1.34(-2)			1	
CH_3COO $\rightarrow \text{CH}_3\text{COOH} +$ (a)							
$\rightarrow \text{CH}_3\text{COOH} +$ (b)							
3-Cyclohexen-1-yl acetate \rightarrow Acetic acid + 1,3-Cyclohexadiene (a) \rightarrow Acetic acid + 1,4-Cyclohexadiene (b)							
72 TIN/KOO ¹⁾	EX	578-653	3.98(11)	0	19527±503	1	2.0
$k_a + k_b$. 72 TIN/KOO ¹⁾ k_b/k_a . ¹⁾ Thermolysis.	RL	637	1.3(1)			1/1	

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}=\text{CH}_2$							
5-Hexen-1-ol acetate							
79 MAR/HER Pyrolysis in a static system. P = (44-282) torr.	EX	513-693	2.69(12)	0	23756±217	1	1.38
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}=\text{C}(\text{CH}_3)_2$ $\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}=\text{C}(\text{CH}_3)_2$ (a) $\rightarrow \text{CH}_3\text{COOH} + \text{cis-CH}_3\text{CH}=\text{CHC}(\text{CH}_3)=\text{CH}_2$ (b) $\rightarrow \text{CH}_3\text{COOH} + \text{trans-CH}_3\text{CH}=\text{CHC}(\text{CH}_3)=\text{CH}_2$ (c) $\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{CHCH}_2\text{C}(\text{CH}_3)=\text{CH}_2$ (d)							
3-Penten-1-ol, 4-methyl-, acetate							
81 CHU/MAR $k_a + k_b + k_c + k_d$. Pyrolysis. Static system. IR-, and NMR-spectrometry. P = (53-210) torr.	EX	603-653	1.62(13)	0	24008±204	1	1.38
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{CH}=\text{CH}_2$ $\rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}(\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2)$ (a) $\rightarrow \text{CH}_3\text{C}(\text{O})\text{H} + (\text{CH}_3)_2\text{C}=\text{CHCH}=\text{CH}_2$ (b)							
4-Penten-2-ol, 2-methyl-, acetate							
79 MAR/HER $k_a + k_b$. Pyrolysis in a static system. P = (44-282) torr.	EX	513-693	3.89(13)	0	20436±349	1	2.0
CH_3COO  $\rightarrow \text{CH}_3\text{COOH} +$ 							
Acetic acid cyclohexyl ester (Dicyclohexyl acetate) \rightarrow Acetic acid + Cyclohexene							
72 TIN/KOO Thermolysis.	EX	613-688	3.16(13)	0	23553±503	1	2.0
 $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}=\text{C}(\text{CH}_3)_2 + \text{CH}_2=\text{C}=\text{O}$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{OCH}=\text{CH}_2 + (\text{CH}_3)_2\text{C}=\text{C}=\text{O}$ (b)							
Cyclobutanone, 3-ethoxy-2,2-dimethyl-							
73 EGG2 1) $k_a + k_b$. Based on internal standard technique.	EX	464-558	3.80(13)	0	20267±342	1	1.95
73 EGG2 1) $k_a + k_b$. Based on measurement of amounts of the ethers formed.	EX	464-558	4.07(13)	0	20292±257	1	1.66
¹) Thermolysis in a static system. P-independent for: $P_0 = (5-50)$ torr. and $P(\text{Total}) < 700$ torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$ \begin{array}{c} \text{CH}_3 \\ \\ \text{C} - \text{COOH} \\ / \quad \backslash \\ \text{CH}_2 \quad \text{CH}_2 \end{array} \rightarrow \text{CH}_3\text{CH}_2\text{C}(\text{CH}_3)=\text{C}(\text{CH}_3)_2 + \text{CO}_2 $						
Cyclopropaneacetic acid, $\alpha, \alpha, 1$ -trimethyl-						
→ 2-Pentene, 2,3-dimethyl-, + Carbon dioxide						
79 BIG/FET ¹⁾	EX	725	(2.63±0.15)(-2)			1
79 BIG/FET ¹⁾	EX	690-740	(3.32±0.21)(11)	0	21871±505	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a Flow-reactor with sealed tubes.						
$ \begin{array}{c} \text{CH}_3 \\ \\ \text{H}_3\text{C} - \text{C} - \text{COOCH}_2\text{CH}_3 \\ / \quad \backslash \\ \text{CH}_2 \quad \text{CH}_2 \end{array} \rightarrow \begin{array}{c} \text{CH}_3 \\ \\ \text{H}_3\text{C} - \text{C} \\ / \quad \backslash \\ \text{CH}_2 \quad \text{COOCH}_2\text{CH}_3 \end{array} $						
Cyclopropanecarboxylic acid, 2,3-dimethyl-						
ethyl ester, (1 α , 2 α , 3 α)-						
→ Cyclopropanecarboxylic acid, 2,3-dimethyl-						
ethyl ester, (1 α , 2 α , 3 β)						
77 GAJ/WEB	EX	503-548	7.24(11)	0	20081±352	1
Thermal isomerization in a static reactor.						
$ \begin{array}{c} \text{CH}_3 \\ \\ \text{H}_3\text{C} - \text{C} \\ / \quad \backslash \\ \text{CH}_2 \quad \text{COOCH}_2\text{CH}_3 \end{array} \rightarrow \begin{array}{c} \text{CH}_3 \\ \\ \text{H}_3\text{C} - \text{C} - \text{COOCH}_2\text{CH}_3 \\ / \quad \backslash \\ \text{CH}_2 \quad \text{CH}_2 \end{array} $						
Cyclopropanecarboxylic acid, 2,3-dimethyl-						
ethyl ester, (1 α , 2 α , 3 β)-						
→ Cyclopropanecarboxylic acid, 2,3-dimethyl-						
ethyl ester, (1 α , 2 α , 3 α)						
77 GAJ/WEB	EX	503-548	7.24(11)	0	21540±352	1
Thermal isomerization in a static reactor.						
$ \text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{CH}_2\text{C}(\text{O})\text{CH}_3 $						
→ CH ₃ COOH + CH ₃ C(O)CH ₂ C(CH ₃)=CH ₂ (a)						
→ CH ₃ COOH + (CH ₃) ₂ C=CHC(O)CH ₃ (b)						
2-Pentanone, 4-(acetyloxy)-4-methyl-						
72 TIN/KOO	EX	498-563	2.00(12)	0	19326±755	1 3.98
k _a .						
Thermolysis.						
72 TIN/KOO	EX	498-563	1.58(11)	0	16205±503	1 2.51
k _b .						
Thermolysis.						
$ \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 $						
→ CH ₃ CH ₂ CH ₂ CH ₂ COOH + CH ₃ CH=CH ₂						
Pentanoic acid 1-methylethyl ester						
77 SMI/MUT	EX	651	(5.97±0.07)(-3)			1

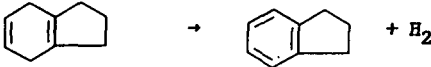
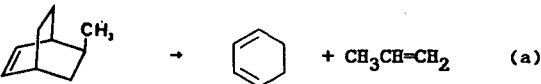
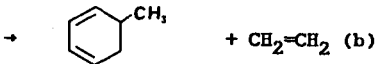
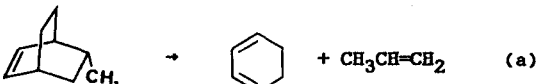

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\text{CH}_3\text{C}(\text{O})\text{OCH}_2\text{CH}_2\text{C}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}(\text{CH}_3)_3$							
1-Butanol, 3,3-dimethyl-, acetate							
79 CHU/MAR Pyrolysis in a static system. P = (63-250) torr.	EX	633-693	2.19(12)	0	23347±505	1	2.24
79 TAY Pyrolysis in a stainless-steel reactor.	EX	660-712	2.24(12)	0	23352	1	
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{CH}_3)\text{C}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{COOH} + (\text{CH}_3)_3\text{CCH}=\text{CH}_2$							
2-Butanol, 3,3-dimethyl-, acetate							
72 CHU/MAR Static system pyrolysis. P = (25-300) torr.	EX	578-653	3.16(12)	0	22174±302	1	1.66
$(\text{CH}_3)_2\text{CHCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_2\text{CHCH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Butanoic acid, 3-methyl-, 1-methylethyl ester							
78 CHU/MAR ¹⁾	EX	603	3.95(-4)			1	
78 CHU/MAR ¹⁾	EX	599-629	1.02(13)	0	22798±201	1	1.35
¹⁾ Pyrolysis in a static system. Gas-chromatography.							
$(\text{CH}_3)_3\text{CC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_3\text{CCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$							
Propanoic acid, 2,2-dimethyl-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(7.68±0.32)(-3)			1	
78 TAY Pyrolysis.	EX	609-667	1.07(13)	0	22562	1	
$\text{CH}_3\text{OCOO}(\text{CH}_2)_5\text{CH}_3 \rightarrow \text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$							
Carbonic acid hexyl methyl ester							
72 BIG/WRE3	EX	629	1.13			1	
72 BIG/WRE3 Flow-tube method. Assumed T-range, omitted in text. The A-factor recalculated from the reported experimental data.	EX	593-648	7.91(15)	0	22949	1	
$\text{CH}_3\text{OC}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$							
→ $\text{CH}_3\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ (a)							
→ $\text{CH}_3\text{OH} + \text{CO}_2 + \text{cis-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3$ (b)							
→ $\text{CH}_3\text{OH} + \text{CO}_2 + \text{trans-CH}_3\text{CH}=\text{CHCH}_2\text{CH}_2\text{CH}_3$ (c)							
Carbonic acid methyl 1-methylpentyl ester							
72 BIG/WRE3	EX	629	3.53(-2)			1	

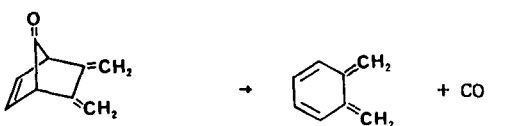
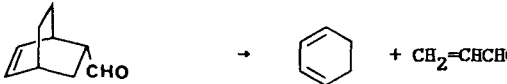
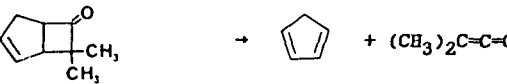
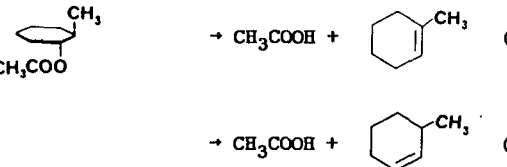
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
72 BIG/WRE3 $k_a + k_b + k_c$. Flow-tube method. Assumed T-range, omitted in text. The A-factor recalculated from the reported experimental data.	EX	598-648	1.91(13)	0	21339	1	
$(\text{CH}_3)_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$							
→ $(\text{CH}_3)_3\text{CO} + (\text{CH}_3)_3\text{CO}$ (a)							
→ $(\text{CH}_3)_2\text{CO} + (\text{CH}_3)_2\text{CO} + \text{CH}_3 + \text{CH}_3$ (b)							
Peroxide, bis(1,1-dimethylethyl)-							
71 CAD/TRO k_a .	EX	373-423	7.94(14)	0	17922±890	1	9.33
79 SEL/WAD k_a . Thermolysis in a static system.	EX	410	(5.30±0.04)(-5)			1	
80 KNO/RIC k_a . Thermolysis of Azomethane and di-t-Butyl peroxide. Mass-spectrometry.	EX	413	(8.9±1.0)(-5)			1	
81 ALA/SEL k_a . Thermolysis in a Pyrex vessel. Static system. Mass-spectrometry.	EX	399-434	7.94(15)	0	19246±349	1	2.0
73 PER/GOL k_p . Limiting high-pressure k. RRKM data-fit.	EX	500-660	3.98(15)	0	18822±503	1	
$(\text{CH}_3)_3\text{CSC}(\text{CH}_3)_3 \rightarrow \text{products}$							
Propane, 2,2'-thiobis[2-methyl- (di-t-Butyl sulfide)							
80 MAR/BAR Uninhibited pyrolysis in a static reactor. The products are: Isobutene, Hydrogen sulfide, Isobutane and t-Butylthiol. P = (26-206) torr.	EX	633-686	1.26(15)	0	27545±962	1	
$(\text{CH}_3)_2\text{C}(\text{N}=\text{N})\text{CH}_2\text{CH}(\text{CH}_3)_2 \rightarrow \text{products}$							
Diazene, bis(2-methylpropyl)-							
78 MCK/TUR 1,1'-Azoisobutane pyrolysis.	EX	553-602	9.12(15)	0	25043±265	1	1.58
$(\text{CH}_3)_3\text{CN}=\text{NC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{C} + (\text{CH}_3)_3\text{C} + \text{N}_2$							
Diazene, bis(1,1-dimethylethyl)-							
73 PER/BEA RRKM fit of experimental data.	EX	503-730	2.51(16)	0	21540±503	1	
77 MAR/MAC ¹⁾	EX	483-533	3.98(15)	0	20448±361	1	2.0
77 MCK/TUR ¹⁾	EX	471-531	8.71(15)	0	21086±355	1	2.09



4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 1H-Indene, 2,3,4,7-tetrahydro- → 1H-Indene, 2,3-dihydro- + Hydrogen molecule 72 COC/FRE Pyrolysis in a static system. P ₀ < 0.8 torr.	EX	619-681	8.91(12)	0	24449±237	1	1.45
 (a)  (b)							
Bicyclo[2.2.2]oct-2-ene, 5-methyl-, (1α,4α,5α)- (exo form) → 1,3-Cyclohexadiene + 1-Propene (a) → 1,3-Cyclohexadiene, 5-methyl- + Ethene (b) 75 HUY/NGO ¹⁾ k _a .	EX	608-679	5.37(14)	0	29265±40	1	1.07
75 HUY/NGO ¹⁾ k _b .	EX	608-679	1.20(15)	0	29774±40	1	1.07
¹⁾ Pyrolysis in a cylindrical Pyrex vessel. Gas-chromatography. P = (7-37) torr.							
 (a)  (b)							
Bicyclo[2.2.2]oct-2-ene, 5-methyl-, (1α,4α,5β)- (endo form) → 1,3-Cyclohexadiene + 1-Propene (a) → 1,3-Cyclohexadiene, 5-methyl-, + Ethene (b) 75 HUY/NGO ¹⁾ k _a .	EX	608-679	1.74(14)	0	28163±30	1	1.05
75 HUY/NGO ¹⁾ k _b .	EX	608-679	1.20(14)	0	28138±40	1	1.07
¹⁾ Pyrolysis in a cylindrical Pyrex vessel. Gas-chromatography. P = (7-37) torr.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 <p>Bicyclo[2.2.1]hept-2-en-7-one, 5,6-bis(methylene)- (o-Quinodimethane) → 1,3-Cyclohexadiene, 5,6-bis(methylene)- + Carbon monoxide</p>	EX	556-638	(3.1±2.9)(13)	0	12884±554	1
<p>81 ROT/SCH M = N₂, or He. Thermolysis. Incident shock-waves. [o-Quinodimethane] ≈ 0.05% (He, N₂)</p>						
 <p>Bicyclo[2.2.2]oct-5-ene-2-carboxaldehyde, (1α,2β,4α)- (endo form) → 1,3-Cyclohexadiene + 2-Propenal (Acrolein)</p>	EX	565-638	9.55(12)	0	23347±55	1 1.10
<p>76 HUY/FAT Retro-Diels-Alder decomposition in a Pyrex vessel. Gas-chromatography. P = (55-240) torr.</p>						
 <p>Bicyclo[3.2.0]hept-2-en-6-one, 7,7-dimethyl- → 1,3-Cyclopentadiene + 1-Propanone, 2-methyl-</p>	EX	470-550	7.94(12)	0	18978±262	1 1.66
<p>73 EGG1 Thermolysis in a static system. Gas-chromatography. P₀ = (7-68) torr.</p>						
 <p>Cyclohexanol, 2-methyl-acetate, (1R-trans)- → Acetic acid + Cyclohexene, 1-methyl- (a) → Acetic acid + Cyclohexene, 3-methyl- (b)</p>	EX	623-688	2.51(13)	0	23553±503	1 2.51
<p>72 TIN/KOO¹⁾ k_a + k_b.</p>	EX	623-688	2.51(13)	0	23553±503	1 2.51
<p>72 TIN/KOO¹⁾ k_a/k_b.</p>	RL	637	1.2			1/1
<p>¹⁾ Thermolysis.</p>						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
<chem>CC(=O)OC1CCCCC1</chem> $\rightarrow \text{CH}_3\text{COOH} +$  (a)							
$\rightarrow \text{CH}_3\text{COOH} +$  (b)							
Cyclohexanol, 2-methyl-acetate, (1S-cis)-							
→ Acetic acid + Cyclohexene, 1-methyl- (a)							
→ Acetic acid + Cyclohexene, 3-methyl- (b)							
72 TIN/KOO ¹⁾	EX	623-688	6.31(13)	0	24157±503	1	3.98
$k_a + k_b$.							
72 TIN/KOO ¹⁾	RL	637	8.6(-1)			1/1	
k_b/k_a .							
1) Thermolysis.							
<chem>CC(=O)OC(C)CC(C)C</chem>							
→ <chem>CC(=O)O</chem> + <chem>CC=C(C)CC(C)C</chem> (a)							
→ <chem>CC(=O)O</chem> + <i>cis</i> - <chem>CC(C)=CC(C)C</chem> (b)							
→ <chem>CC(=O)O</chem> + <i>trans</i> - <chem>CC(C)=CC(C)C</chem> (c)							
2-Pentanol, 2,4-dimethyl-, acetate							
79 TAY	RL	673	1.85			1/1	
$k_a/(k_b + k_c)$. Pyrolysis in a stainless-steel reactor. Gas-chromatography. The % of alkene-1 and alkene-2 reported in the text (61.5 and 38.5 respectively) give a ratio of only 1.60.							
<chem>CC(=O)OC(C)CC(C)(C)C</chem>							
→ <chem>CC(=O)O</chem> + <chem>CC=CC(C)C(C)C</chem> (a)							
→ <chem>CC(=O)O</chem> + <i>cis</i> - <chem>CC(C)=CC(C)C</chem> (b)							
→ <chem>CC(=O)O</chem> + <i>trans</i> - <chem>CC(C)=CC(C)C</chem> (c)							
2-Pentanol, 4,4-dimethyl-, acetate							
79 TAY	RL	668-778	4.9(-1)			1/1	
$k_a/(k_b + k_c)$. Pyrolysis in a stainless-steel reactor. Gas-chromatography.							
81 CHU/DOM	EX	573-623	7.41(14)	0	21796±409	1	2.04
$k_a + k_b + k_c$. Pyrolysis in a static system. NMR-spectroscopy. P = (48-211) torr.							
<chem>CC(=O)OC(C)CC(C)(C)C</chem> → <chem>CC(=O)O</chem> + <chem>CC(C)C=CC</chem>							
3-Pentanol, 2,2-dimethyl-, acetate							
72 CHU/MAR	EX	578-653	1.15(13)	0	22572±393	1	1.23
Pyrolysis in a static system. P = (25-300) torr.							

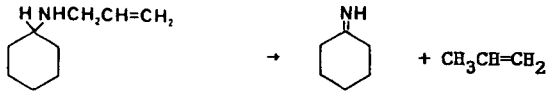
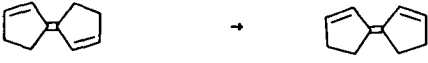

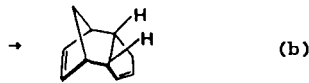
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_3\text{C}(\text{O})\text{OC}[\text{CH}(\text{CH}_3)_2](\text{CH}_3)\text{CH}_2\text{CH}_3$ → $\text{CH}_3\text{COOH} + (\text{CH}_3)_2\text{C}=\text{C}(\text{CH}_3)\text{CH}_2\text{CH}_3$ (a) → $\text{CH}_3\text{COOH} + \text{cis-CH}_3\text{CH}=\text{C}[\text{CH}(\text{CH}_3)_2]\text{CH}_3$ (b) → $\text{CH}_3\text{COOH} + \text{trans-CH}_3\text{CH}=\text{C}[\text{CH}(\text{CH}_3)_2]\text{CH}_3$ (c)						
3-Pentanol, 2,3-dimethyl-, acetate 77 CUE/CHU $k_a + k_b + k_c$	EX	485-533	1.66(14)	0	20433±252	1 1.69
$\text{CH}_3\text{C}(\text{O})\text{OC}(\text{CH}_3)_2\text{C}(\text{CH}_3)_3 \rightarrow \text{CH}_3\text{COOH} + \text{CH}_2=\text{C}(\text{CH}_3)\text{C}(\text{CH}_3)_3$ 2-Butanol, 2,3,3-trimethyl-, acetate 80 MAR/CHU Pyrolysis. Static system. P = (56-210) torr.	EX	503-513	2.51(14)	0	20629±553	1 3.09
$(\text{CH}_3)_3\text{CC}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$ Propanoic acid, 2,2-dimethyl-, 1,1-dimethylethyl ester 78 TAY Pyrolysis.	EX	519-608	1.05(13)	0	19884	1
$(\text{CH}_3\text{CH}_2)_2\text{CHC}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3\text{CH}_2)_2\text{CHCOOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Butanoic acid, 2-ethyl-, 1-methylethyl ester 77 SMI/MUT	EX	651	(6.97±0.17)(-3)			1
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow (\text{CH}_3)_3\text{CCH}_2\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Butanoic acid, 3,3-dimethyl-, 1-methylethyl ester 77 SMI/MUT 78 CHU/MAR Pyrolysis in a static system.	EX	651	(5.95±0.19)(-3)			1
	EX	589-628	4.47(13)	0	23704±324	1 1.74
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2$ → $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}(\text{CH}_3)\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Pentanoic acid, 2-methyl-, 1-methylethyl ester 77 SMI/MUT	EX	651	(6.88±0.24)(-3)			1
$\text{CH}_3(\text{CH}_2)_4\text{C}(\text{O})\text{OCH}(\text{CH}_3)_2 \rightarrow \text{CH}_3(\text{CH}_2)_4\text{COOH} + \text{CH}_3\text{CH}=\text{CH}_2$ Hexanoic acid 1-methylethyl ester 77 SMI/MUT	EX	651	(6.03±0.27)(-3)			1
$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ → $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ Carbonic acid dibutyl ester (Di-n-butyl carbonate) 72 BIG/WRE1 ¹) Sealed-tube pyrolysis.	EX	554-594	1.32(12)	0	21892	1

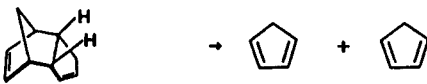
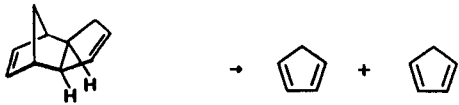
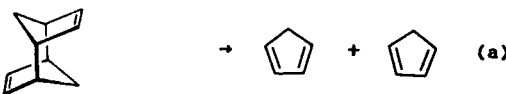
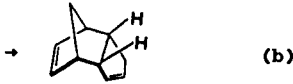
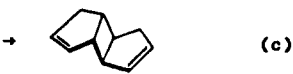
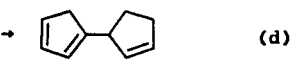
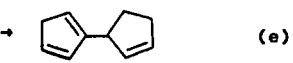
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
72 BIG/WRE1 ¹⁾	EX	700	(9.70±0.29)(-2)			1
72 BIG/WRE1 ¹⁾	EX	663-708	(1.56±0.05)(13)	0	22899	1
Flow-tube pyrolysis.						
The A-factor recalculated from the reported data.						
¹⁾ Pyrolysis in Kooyman, or break-seal tubes.						
$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)\text{OC}(\text{O})\text{OCH}(\text{CH}_3)\text{CH}_2\text{CH}_3$						
→ $\text{CH}_3\text{CH}_2\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$ (a)						
→ <i>cis</i> - $\text{CH}_3\text{CH}=\text{CHCH}_3 + \text{CO}_2 + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$ (b)						
→ <i>trans</i> - $\text{CH}_3\text{CH}=\text{CHCH}_3 + \text{CO}_2 + \text{CH}_3\text{CH}(\text{OH})\text{CH}_2\text{CH}_3$ (c)						
Carbonic acid bis(1-methylpropyl) ester (Di- <i>n</i> -butyl carbonate)						
72 BIG/WRE2 ¹⁾	EX	629	5.25(-2)			1
Flow-tube pyrolysis.						
72 BIG/WRE2 ¹⁾	EX	593-648	1.50(13)	0	20936	1
Flow-tube pyrolysis.						
The A-factor recalculated from the reported data.						
72 BIG/WRE2 ¹⁾	EX	629	6.09(-2)			1
Sealed-tube pyrolysis.						
72 BIG/WRE2 ¹⁾	EX	489-540	9.07(12)	0	20533	1
Sealed-tube pyrolysis.						
¹⁾ Pyrolysis in Kooyman, or break-seal tubes.						
$(\text{CH}_3)_2\text{CHCH}_2\text{OC}(\text{O})\text{OCH}_2\text{CH}(\text{CH}_3)_2$						
→ $(\text{CH}_3)_2\text{C}=\text{CH}_2 + \text{CO}_2 + (\text{CH}_3)_2\text{CHCH}_2\text{OH}$						
Carbonic acid bis(2-methylpropyl) ester (Di- <i>i</i> -butyl carbonate)						
72 BIG/WRE1 ¹⁾	EX	700	3.2(-1)			1
72 BIG/WRE1 ¹⁾	EX	663-708	(5.53±0.17)(13)	0	24560	1
The A-factor recalculated from the reported data.						
¹⁾ Pyrolysis in the Kooyman flow-tube.						
$(\text{CH}_3)_3\text{COC}(\text{O})\text{OC}(\text{CH}_3)_3 \rightarrow (\text{CH}_3)_3\text{COH} + \text{CO}_2 + (\text{CH}_3)_2\text{C}=\text{CH}_2$						
Carbonic acid bis(1,1-dimethylethyl) ester (Di- <i>t</i> -butyl carbonate)						
72 BIG/WRE3	EX	453-498	2.4(13)	0	19124	1
Sealed-tube.						
72 BIG/WRE3	EX	629	2.01			1
72 BIG/WRE3	EX	593-648	1.31(12)	0	17111	1
Flow-tube. Assumed T-range, omitted in text.						
A-factor recalculated from the reported data.						

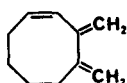
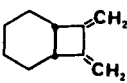

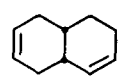
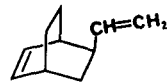


4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$(\text{CH}_2=\text{CHCH}_2)_3\text{N} \rightarrow \text{CH}_2=\text{CHCH}_2\text{N}=\text{CHCH}=\text{CH}_2 + \text{CH}_3\text{CH}=\text{CH}_2$ 2-Propen-1-amine, N,N-di-2-propenyl- (Triallylamine) → 2-Propen-1-amine, N-2-propenylidene- + 1-Propene	74 VII/EGG1	EX 531-620	5.50(11)	0	19260±96	1	1.17
Thermolysis. Static system. N-2-Propenylidene-2-propen-1-amine undergoes cyclization to give 3-Methylpyridine. P(Triallylamine) = (3-36) torr. P(Total) = (23-178) torr.							
	73 EGG3	EX 562-652	2.75(11)	0	21228±287	1	1.62
Cyclohexanamine, N-2-propenyl- → 1-Propene + Cyclohexanimine Thermolysis in a static system. Gas-chromatography. k is P-independent within the given P-range. P = (15-150) torr.							
	73 DOE/BEA	EX 526-576	1.07(12)	0	20986±403	1	2.09
Cyclopentene, 3-(cyclopent-4-en-1-ylidene)- (trans form) → Cyclopentene, 3-(cyclopent-2-en-1-ylidene)- (cis form) Thermal isomerization in a 12 l. Pyrex flask, or in a 3.5 l. Corning lead-potash flask.							
							
							
Tricyclo[5.3.0.0 ^{2,6}]deca-3,9-diene (anti-cis-[2+2]-Dicyclopentadiene) → 1,3-Cyclopentadiene + 1,3-Cyclopentadiene (a) → Tricyclo[5.2.1.0 ^{2,6}]deca-3,8-diene, endo- (endo-[2+4]-Dicyclopentadiene) (b)							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 <p>Tricyclo[5.2.1.0^{2,6}]deca-3,8-diene, endo- (endo-[2+4]-Dicyclopentadiene) → 1,3-Cyclopentadiene + 1,3-Cyclopentadiene</p>	81 GRI/SCH	EX 431-494	(2.0±0.4)(14)	0	18671±101	1
Thermolysis. P = (2-3) torr.						
 <p>Tricyclo[5.2.1.0^{2,6}]deca-3,8-diene, exo- (exo-[2+4]-Dicyclopentadiene) → 1,3-Cyclopentadiene + 1,3-Cyclopentadiene</p>	81 GRI/SCH	EX 481-551	(5.6±0.4)(14)	0	21389±50	1
Thermolysis. P = (2-3) torr.						
 <p>(a)</p>						
 <p>(b)</p>						
 <p>(c)</p>						
 <p>(d)</p>						
 <p>(e)</p>						
<p>Tricyclo[4.2.1.1^{2,5}]deca-3,7-diene, (1α,2β,5β,6α)- (anti-[4+4]-Dicyclopentadiene) → 1,3-Cyclopentadiene + 1,3-Cyclopentadiene (a) → Tricyclo[5.2.1.0^{2,6}]deca-3,8-diene, endo- (b) → Tricyclo[5.3.0.0^{2,6}]deca-3,9-diene (c) → 1,3-Cyclopentadiene, 1-(2-cyclopenten-1-yl)- (d) → 1,3-Cyclopentadiene, 2-(2-cyclopenten-1-yl)- (e)</p>	81 GRI/SCH	EX 460-532	(5.0±0.9)(14)	0	20030±101	1
Thermolysis. P = (2-3) torr.						

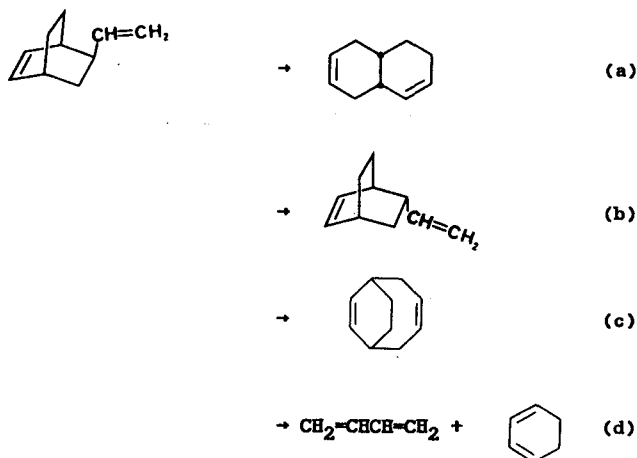
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
$\text{CH}_2=\text{C}=\text{CHCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}=\text{C}=\text{CH}_2 \rightarrow$  (a)						
\rightarrow  (b)						
1,2,8,9-Decatetraene						
→ Cyclooctene, 3,4-bis(methylene)-			(a)			
→ Bicyclo[4.2.0]octane, 7,8-bis(methylene)-, cis-			(b)			
82 GAJ/BEN	EX	633-693	2.5(9)	0	15501	1
$k_a + k_b$. Pyrolysis.						
Flow-system. Intramolecular Allene addition.						
Major product given by (a).						
 →  (a)						
→  (b)						
→  (c)						
→ $\text{CH}_2=\text{CHCH}=\text{CH}_2 +$  (d)						
Bicyclo[4.2.2]deca-3,7-diene						
→ Naphthalene, 1,2,4a,5,8,8a-hexahydro-, cis-			(a)			
→ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 α)- (exo form)			(b)			
→ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 β)- (endo form)			(c)			
→ 1,3-Butadiene + 1,3-Cyclohexadiene			(d)			
82 HUY/HUB1 ¹⁾	EX	456-526	4.37(14)	0	22662±35	1 1.07
k_a . Thermal isomerization.						
82 HUY/HUB1 ¹⁾	EX	456-526	4.17(14)	0	23437±35	1 1.07
k_b . Thermal isomerization.						
82 HUY/HUB1 ¹⁾	EX	456-526	1.41(14)	0	23342±45	1 1.10
k_c . Thermal isomerization.						
82 HUY/HUB1 ¹⁾	EX	456-526	5.25(15)	0	24826±35	1 1.07
k_d . Thermolysis.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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¹) Thermal isomerization, or decomposition
in a static system with cylindrical packed,
or unpacked Pyrex vessels. Gas-chromatography.
NMR-, IR-, and Mass-spectrometry.
P₀ = (2-40) torr.



Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 α)-
(exo form)

→ Naphthalene, 1,2,4a,5,8,8a-hexahydro-, cis- (a)

→ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-,
(1 α ,4 α ,5 β)- (endo form) (b)

→ Bicyclo[4.2.2]deca-3,7-diene (c)

→ 1,3-Butadiene + 1,3-Cyclohexadiene (d)

82 HUY/HUB1 ¹) EX 513-578 1.05(14) 0 25450±91 1 1.17

k_a. Thermal isomerization.

82 HUY/HUB1 ¹) EX 513-578 9.33(13) 0 25798±101 1 1.20

k_b. Thermal isomerization.

82 HUY/HUB1 ¹) EX 513-578 2.57(13) 0 24731±161 1 1.35

k_c. Thermal isomerization.

82 HUY/HUB1 ¹) DE 513-578 8.91(14) 0 26694±50 1 1.10

k_a. Thermolysis.

Calculated by combining several k's measured
in this work with their respective equilibrium
constants.

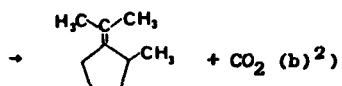
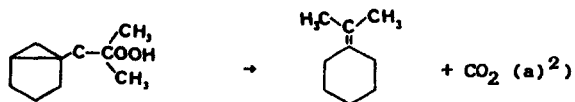
¹) Thermal isomerization, or decomposition
in a static system with cylindrical packed,
or unpacked Pyrex vessels. Gas-chromatography.
NMR-, IR-, and Mass-spectrometry.
P₀ = (2-40) torr.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
→			(a)			
→			(b)			
→			(c)			
→ CH ₂ =CHCH=CH ₂ +			(d)			
Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 β)- (endo form)						
→ Naphthalene, 1,2,4a,5,8,8a-hexahydro, cis-	(a)					
→ Bicyclo[2.2.2]oct-2-ene, 5-ethenyl-, (1 α ,4 α ,5 α)- (exo form)	(b)					
→ Bicyclo[4.2.2]deca-3,7-diene	(c)					
→ 1,3-Butadiene + 1,3-Cyclohexadiene	(d)					
82 HUY/HUB1 ¹⁾ k _a . Thermal isomerization.	EX	476-563	8.91(12)	0	22416±60	1 1.12
82 HUY/HUB1 ¹⁾ k _b . Thermal isomerization. Calculated by combining several k's measured in this work with their respective equilibrium constants.	DE	476-563	8.91(13)	0	25949±292	1 1.70
82 HUY/HUB1 ¹⁾ k _c . Thermal isomerization. Calculated by combining several k's measured in this work with their respective equilibrium constants.	DE	476-563	8.13(12)	0	24791±232	1 1.51
82 HUY/HUB1 ¹⁾ k _d . Thermolysis.	EX	476-563	2.88(14)	0	25908±101	1 1.20
¹⁾ Thermolysis in a static system with cylindrical packed, or unpacked Pyrex vessels. Gas-chromatography. P ₀ = (2-40) torr.						
CH ₃ (CH ₂) ₈ CH ₃ → products						
Decane						
71 GON/LEW	EX	713-793	1.95(3)	0	13337	1
80 RUM/SHE	EX	918-958	2.19(14)	0	31274±4126	1 11.22
Pyrolysis in a quartz reactor. P = 760 torr.						

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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Bicyclo[3.1.0]hexane-1-acetic acid, α, α -dimethyl-

→ Cyclohexane, (1-methylethylidene)-

+ Carbon dioxide (a)

→ Cyclopentane, 1-methyl-2-(1-methylethylidene)-

+ Carbon dioxide (b)

79 BIG/FET ¹⁾ k _a .	EX	725 [*]	1.56(-2)			1
79 BIG/FET ¹⁾ k _b .	EX	725	9.7(3)			1
79 BIG/FET ¹⁾ k _a + k _b .	EX	725	(2.53±0.10)(-2)			1
79 BIG/FET ¹⁾ k _a + k _b .	EX	690-740	(9.21±0.36)(10)	0	20969±806	1

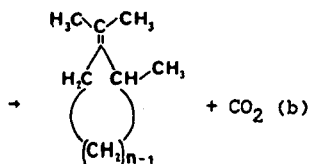
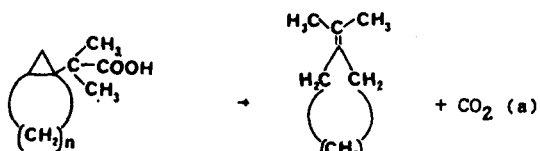
A and B recalculated from the reported experimental data.

¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed tubes.

Gas-chromatography.

NMR-spectroscopy.

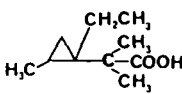
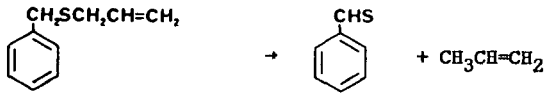
²⁾ The general mechanism of this type of reaction is:



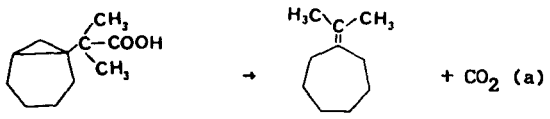
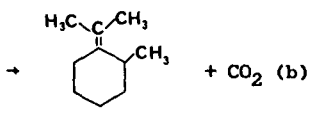

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k(k(ref)), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
$\begin{array}{c} \text{CH}_3\text{COO} \\ \\ \text{Cyclohexane ring} \\ \\ \text{CH}_3\text{COO} \end{array} \rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{CH}_3\text{COO} \\ \\ \text{Cyclohexene ring} \end{array} \quad (\text{a})$							
$\begin{array}{c} \text{CH}_3\text{COO} \\ \\ \text{Cyclohexane ring} \\ \\ \text{CH}_3\text{COO} \end{array} \rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{CH}_3\text{COO} \\ \\ \text{Cyclohexene ring} \end{array} \quad (\text{b})$							
1,2-Cyclohexanediol diacetate, trans-							
→ Acetic acid + 1-Cyclohexen-1-ol acetate (a)							
→ Acetic acid + 2-Cyclohexen-1-ol acetate (b)							
72 TIN/KOO ¹⁾	EX	643-733	3.16(12)	0	24006±503	1	2.0
$k_a + k_b$.							
72 TIN/KOO ¹⁾	RL	637	4.0(-1)				1/1
k_a/k_b .							
¹⁾ Thermolysis.							
$\begin{array}{c} \text{CH}_3\text{COO} \\ \\ \text{Cyclohexane ring} \\ \\ \text{CH}_3\text{COO} \end{array} \rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{CH}_3\text{COO} \\ \\ \text{Cyclohexene ring} \end{array} \quad (\text{a})$							
$\begin{array}{c} \text{CH}_3\text{COO} \\ \\ \text{Cyclohexane ring} \\ \\ \text{CH}_3\text{COO} \end{array} \rightarrow \text{CH}_3\text{COOH} + \begin{array}{c} \text{CH}_3\text{COO} \\ \\ \text{Cyclohexene ring} \end{array} \quad (\text{b})$							
1,2-Cyclohexanediol diacetate, cis-							
→ Acetic acid + 1-Cyclohexen-1-ol acetate (a)							
→ Acetic acid + 2-Cyclohexen-1-ol acetate (b)							
72 TIN/KOO ¹⁾	EX	643-733	5.01(12)	0	24157±1510	1	3.16
$k_a + k_b$.							
72 TIN/KOO ¹⁾	RL	637	1.46(-1)				1/1
k_b/k_a .							
¹⁾ Thermolysis.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}(\text{C}(\text{CH}_3)_3)\text{CH}_2\text{CH}=\text{CH}_2$							
→ $\text{CH}_3\text{COOH} + \text{cis}-(\text{CH}_3)_3\text{CCH}=\text{CHCH}=\text{CH}_2$ (a)							
→ $\text{CH}_3\text{COOH} + \text{trans}-(\text{CH}_3)_3\text{CCH}=\text{CHCH}=\text{CH}_2$ (b)							
5-Hexen-3-ol, 2,2-dimethyl-, acetate							
→ 1,3-Hexadiene, 5,5-dimethyl-, (Z)- (a)							
→ 1,3-Hexadiene, 5,5-dimethyl-, (E)- (b)							
73 CHU/PIO	EX	573-623	1.38(14)	0	23352±302	1	1.02
$k_a + k_b$.							
Pyrolysis in a static system.							
P = (35-300) torr.							

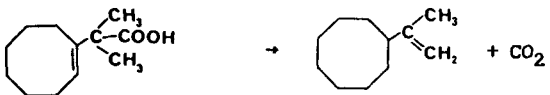
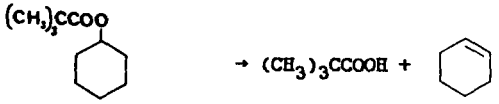
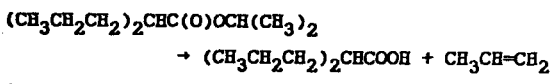
4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
 $\rightarrow (\text{CH}_3)_2\text{CHG}(\text{CH}_2\text{CH}_3)=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ (a) $\rightarrow \text{CH}_3\text{CH}_2\text{CH}_2\text{C}(\text{CH}_2\text{CH}_3)=\text{C}(\text{CH}_3)_2 + \text{CO}_2$ (b)							
Cyclopropaneacetic acid, 1-ethyl- $\alpha,\alpha,2$ -trimethyl-							
\rightarrow 2-Pentene, 3-ethyl-2,4-dimethyl- + Carbon dioxide (a)							
\rightarrow 2-Hexene, 3-ethyl-2-methyl- + Carbon dioxide (b)							
79 BIG/FET ¹⁾ k _a = k _b .	EX	725	5.25(-3)				1
79 BIG/FET ¹⁾ k _a + k _b .	EX	725	(1.05±0.10)(-2)				1
79 BIG/FET ¹⁾ k _a + k _b .	EX	690-740	(1.41±0.13)(11)	0	21919±625		1
A and B recalculated from the reported data.							
¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed tubes. Gas-chromatography. NMR-spectroscopy.							
$\text{CH}_3\text{C}(\text{O})\text{OCH}[\text{CH}(\text{CH}_3)_2]\text{C}(\text{CH}_3)_3$ $\rightarrow \text{CH}_3\text{COOH} + (\text{CH}_3)_3\text{CCH}=\text{C}(\text{CH}_3)_2$							
3-Pentanol, 2,2,4-trimethyl-, acetate							
72 CHU/MAR Pyrolysis in a static system. P = (25-300) torr.	EX	578-653	1.32(13)	0	23452±116	1	1.20
$(\text{CH}_3)_3\text{CCH}_2\text{C}(\text{O})\text{OC}(\text{CH}_3)_3$ $\rightarrow (\text{CH}_3)_3\text{CCH}_2\text{COOH} + (\text{CH}_3)_2\text{C}=\text{CH}_2$							
Butanoic acid, 3,3-dimethyl-, 1,1-dimethylethyl ester							
78 TAY Pyrolysis.	EX	558-620	5.24(12)	0	19527	1	
							
Benzene, [(2-propenylthio)methyl]- (Allyl benzyl sulfide)							
\rightarrow Benzenecarbothioaldehyde + 1-Propene							
82 MAR/ROP2 Pyrolysis. Stirred-flow. Benzene carbothioaldehyde [Benzylthioaldehyde] polymerizes into an amorphous solid. P = (2-15) torr.	EX	588-691	8.51(10)	0	16960±241	1	1.51

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

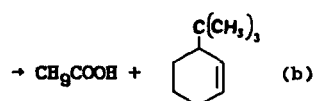
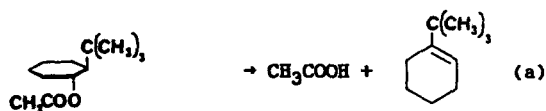
Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
 						
Bicyclo[4.1.0]heptane-1-acetic acid, α, α -dimethyl- → Cycloheptane, (1-methylethylidene)- + Carbon dioxide (a)						
→ Cyclohexane, 1-methyl-2-(1-methylethylidene)- + Carbon dioxide (b)						
79 BIG/FET ¹⁾ k_a .	EX	725	3.09(-2)			1
79 BIG/FET ¹⁾ k_b .	EX	725	8.7(-3)			1
79 BIG/FET ¹⁾ $k_a + k_b$.	EX	725	(3.96±0.16)(-2)			1
79 BIG/FET ¹⁾ $k_a + k_b$.	EX	690-740	(6.81±0.28)(9)	0	18756±854	1
A and B recalculated from the reported data.						
¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed tubes. Gas-chromatography. NMR-spectroscopy. See footnote ²⁾ above for the general mechanism of this type of reaction.						
						
endo-Tricyclo[6.2.2.0 ^{2.7}]dodeca-3,9-diene → 1,3-Cyclohexadiene + 1,3-Cyclohexadiene						
71 DEM/HUY Thermolysis in a Pyrex vessel. P = (4-20) torr.	EX	471-739	2.51(14)	0	26170±956	1 5.01
CH₃(CH₂)₁₀CH₃ → products Dodecane						
80 RUM/SHE Pyrolysis in a quartz reactor. P = 760 torr.	EX	873-953	8.91(13)	0	30216±1010	1 3.02

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
							
1-Cyclooctene-1-acetic acid, α, α -dimethyl- → Cyclooctane, (1-methylethenyl)- + Carbon dioxide							
77 BIG/WEA ¹⁾	RL	500	1.9				1/1
k/k _{ref} : k _{ref} : CH ₃ CH=C(CH ₂ CH ₃)C(CH ₃) ₂ COOH → CH ₃ CH=C(CH ₃ CH ₃)CH(CH ₃) ₂ + CO ₂							
77 BIG/WEA ¹⁾	EX	500	1.66(-4)				1
¹⁾ PYROLYSIS in a flow-reactor. Gas-chromatography.							
							
Propanoic acid, 2,2-dimethyl-, cyclohexyl ester (Cyclohexyl pivalate) → Propanoic acid, 2,2-dimethyl- (Pivalic acid) + Cyclohexene							
72 TIN/KOO	EX	613-663	1.0(13)	0	22647±1007	1	5.01
Thermolysis.							
CH ₃ CH ₂ C(CH ₃) ₂ OOC(CH ₃) ₂ CH ₂ CH ₃ → products Peroxide, bis(1,1-dimethylpropyl)-							
73 PER/GOL	EX	523-633	6.31(15)	0	18319±503	1	
A and B factors recommended for T = 300 K. Limiting high-pressure k. RRKM data-fit.							
							
Pentanoic acid, 2-propyl-, 1-methylethyl ester							
77 SMI/MUT	EX	651	(6.89±0.30)(-3)				1
CH ₃ CH ₂ C(CH ₃) ₂ OC(O)OC(CH ₃) ₂ CH ₂ CH ₃ → CH ₃ CH ₂ C(CH ₃) ₂ OH + CO ₂ + CH ₂ =C(CH ₃)CH ₂ CH ₃ (a) → CH ₃ CH ₂ C(CH ₃) ₂ OH + CO ₂ + (CH ₃) ₂ C=CHCH ₃ (b)							
Carbonic acid bis(1,1-dimethylpropyl) ester							
72 BIG/WRE3	EX	629	4.05				1
72 BIG/WRE3	EX	593-648	1.03(13)	0	17967	1	
k _a + k _b . Flow-tube method. Assumed T-range, omitted in text. A and B recalculated from the reported data.							

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A units	k err. factor
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Cyclohexanol, 2-(1,1-dimethylethyl)-acetate, trans-

→ Acetic acid + Cyclohexene,

1-(1,1-dimethylethyl)- (a)

→ Acetic acid + Cyclohexene,

3-(1,1-dimethylethyl)- (b)

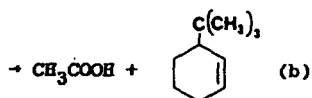
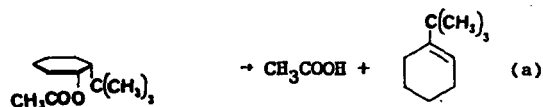
72 TIN/KOO ¹⁾ EX 588-643 6.31(13) 0 22144±1510 1 10.0

$k_a + k_b$.

72 TIN/KOO ¹⁾ RL 637 3.0 1/1

k_a/k_b .

¹⁾ Thermolysis.



Cyclohexanol, 2-(1,1-dimethylethyl)-acetate, cis-

→ Acetic acid + Cyclohexene,

1-(1,1-dimethylethyl)- (a)

→ Acetic acid + Cyclohexene,

3-(1,1-dimethylethyl)- (b)

72 TIN/KOO ¹⁾ EX 618-688 1.26(13) 0 23654±1007 1 5.01

$k_a + k_b$.

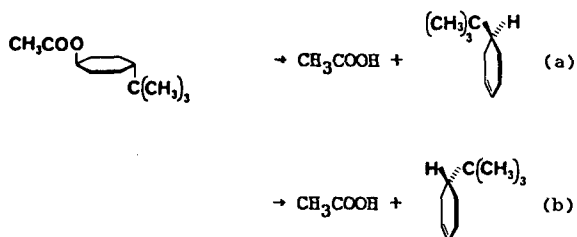
72 TIN/KOO ¹⁾ RL 637 1.20 1/1

k_b/k_a .

¹⁾ Thermolysis.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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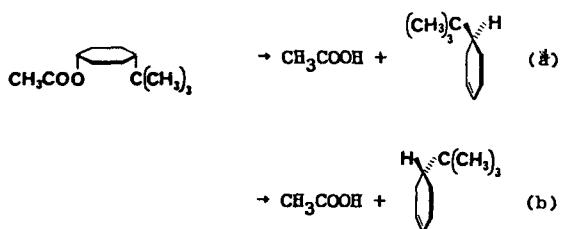


Cyclohexanol, 4-(1,1-dimethylethyl)-acetate, trans-

- Acetic acid + Cyclohexene,
4-(1,1-dimethylethyl)- (R), (a)
- Acetic acid + Cyclohexene,
4-(1,1-dimethylethyl)- (S), (b)

72 TIN/KOO ¹⁾ k _a + k _b .	EX	618-698	1.26(12)	0	21641±1510	1 10.0
72 TIN/KOO ¹⁾ k _a /k _b .	RL	637	1.0			1/1

¹⁾ Thermolysis.



Cyclohexanol, 4-(1,1-dimethylethyl)-acetate, cis-

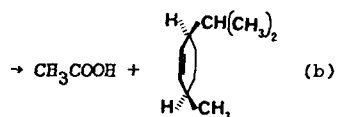
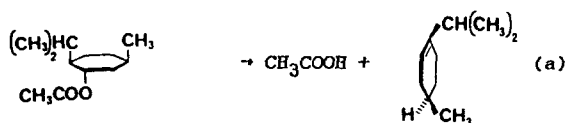
- Acetic acid + Cyclohexene,
4-(1,1-dimethylethyl)-, (R)- (a)
- Acetic acid + Cyclohexene,
4-(1,1-dimethylethyl)-, (S)- (b)

72 TIN/KOO ¹⁾ k _a + k _b .	EX	618-698	3.16(12)	0	21641±1510	1 10.0
72 TIN/KOO ¹⁾ k _a /k _b .	RL	637	1.0			1/1

¹⁾ Thermolysis.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
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Cyclohexanol, 5-methyl-2-(1-methylethyl)-
acetate, (1 α , 2 β , 5 β)-
(trans-2-Isopropyl-1-menthyl acetate)
→ Acetic acid + Cyclohexene, 4-methyl-
1-(1-methylethyl)- (a)
→ Acetic acid + Cyclohexene, 3-methyl-
5-(1-methylethyl)-, cis- (b)

72 TIN/KOO ¹⁾

EX 598-673 5.01(12) 0 21943±503 1 2.0

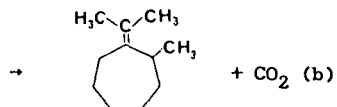
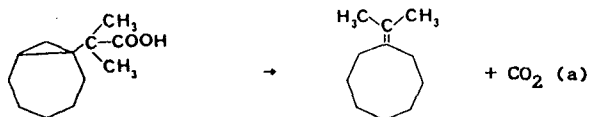
$k_a + k_b$.

72 TIN/KOO ¹⁾

RL 637 1.8 1/1

k_a/k_b .

¹⁾ Thermolysis. The reactant exists in two forms:
5 α and 5 β , not specified in the text. Only the
form 5 β is given here.



Bicyclo[5.1.0]octane-1-acetic acid, α,α -dimethyl-
→ Cyclooctane, (1-methylethylidene)-
+ Carbon dioxide (a)
→ Cycloheptane, 1-methyl-2-(1-methylethylidene)-
+ Carbon dioxide (b)

79 BIG/FET ¹⁾

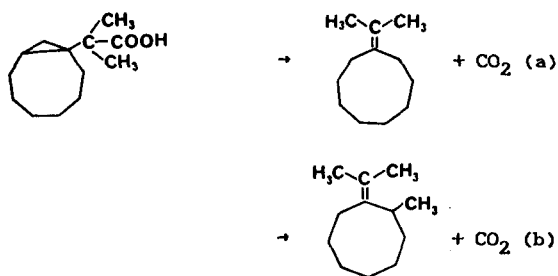
EX 725 4.56(-2) 1

k_a .

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k, k/k(ref), A, A/A(ref)	n	B, B-B(ref)	k, A k err. units factor
79 BIG/FET ¹⁾ k _b .	EX	725	5.3(-3)			1
79 BIG/FET ¹⁾ k _a + k _b .	EX	725	(5.09±0.21)(-2)			1
79 BIG/FET ¹⁾ k _a + k _b . A and B recalculated from the reported data.	EX	690-740	(3.82±0.16)(9)	0	18154±758	1

¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed tubes.
Gas-chromatography.
NMR-spectroscopy.
See footnote ²⁾ above for the general mechanism of this type of reaction.



Bicyclo[6.1.0]nonane-1-acetic acid, α, α -dimethyl-
 → Cyclononane, (1-methylethylidene)-
 + Carbon dioxide (a)
 → Cyclooctane, 1-methyl-2-(1-methylethylidene)-
 + Carbon dioxide (b)

79 BIG/FET ¹⁾ k _a .	EX	725	5.67(-2)			1
79 BIG/FET ¹⁾ k _b .	EX	725	4.8(-3)			1
79 BIG/FET ¹⁾ k _a + k _b .	EX	725	(6.15±0.19)(-2)			1
79 BIG/FET ¹⁾ k _a + k _b . A and B recalculated from the reported data.	EX	690-740	(2.95±0.09)(9)	0	17829±1107	1

¹⁾ Pyrolysis in a Flow-reactor with evacuated sealed tubes.
Gas-chromatography.
NMR-spectroscopy.
See footnote ²⁾ above for the general mechanism of this type of reaction.

4. Table of Chemical Kinetic Data for Combustion Chemistry -- Continued

Reaction, Reference Code, Notes	Data type	T/K	k,k/k(ref), A,A/A(ref)	n	B, B-B(ref)	k,A k err. units factor
$\text{CH}_3(\text{CH}_2)_5\text{OC}(\text{O})\text{O}(\text{CH}_2)_5\text{CH}_3$ $\rightarrow \text{CH}_3(\text{CH}_2)_5\text{OH} + \text{CO}_2 + \text{CH}_2=\text{CH}(\text{CH}_2)_3\text{CH}_3$						
Carbonic acid dihexyl ester (Di-n-hexyl carbonate)						
72 BIG/WRE1 ¹⁾ Sealed-tube pyrolysis.	EX	554-594	4.2(12)	0	22496	1
72 BIG/WRE1 ¹⁾	EX	700	(1.30±0.04)(-1)			1
72 BIG/WRE1 ¹⁾ Flow-tube pyrolysis. The A-factor recalculated from the reported data.	EX	663-708	(7.65±0.23)(12)	0	22194	1
¹⁾ Pyrolysis in Kooyman or break-seal tubes.						
$\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{CH}_3)\text{OC}(\text{O})\text{OCH}(\text{CH}_3)(\text{CH}_2)_3\text{CH}_3$ $\rightarrow \text{CH}_3(\text{CH}_2)_3\text{CH}=\text{CH}_2 + \text{CO}_2 + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$ (a) $\rightarrow \text{cis-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CO}_2$ $\quad\quad\quad + \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$ (b) $\rightarrow \text{trans-CH}_3\text{CH}_2\text{CH}_2\text{CH}=\text{CHCH}_3 + \text{CO}_2$ $\quad\quad\quad \text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}(\text{OH})\text{CH}_3$ (c)						
Carbonic acid bis(1-methylpentyl) ester						
72 BIG/WRE2 $k_a + k_b + k_c$.	EX	629	6.29(-2)			1
72 BIG/WRE2 $k_a + k_b + k_c$. The A-factor recalculated from the reported data.	EX	593-648	6.34(12)	0	20282	1
¹⁾ Flow-tube pyrolysis.						
$\text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{OCH}_2(\text{CH}_2)_5\text{CH}_3$ $\rightarrow \text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{O} + \text{CH}_3(\text{CH}_2)_5\text{CH}_2\text{O}$						
Peroxide, diheptyl-						
82 SAH/RIG Decomposition in a O_2/CO_2 mixture, in a quartz vessel. P(Total) = 180 torr.	EX	509	(6.7±1.4)(-1)			1
$\text{CH}_3(\text{CH}_2)_{13}\text{CH}_3 \rightarrow \text{products}$ Pentadecane						
80 RUM/SHE Pyrolysis in a quartz reactor. P = 760 torr.	EX	888-993	2.95(14)	0	31370±1612	1 6.03

5. References to the Table

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6. Conversion Factors for Rate Constants

Equivalent second order rate constants

A \ B	$\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	$\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1}$	$\text{m}^3 \text{ mol}^{-1} \text{ s}^{-1}$	$\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$	$(\text{mm Hg})^{-1} \text{ s}^{-1}$	$\text{atm}^{-1} \text{ s}^{-1}$	$\text{ppm}^{-1} \text{ min}^{-1}$	$\text{m}^2 \text{ kN}^{-1} \text{ s}^{-1}$
1 $\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1} =$	1	10^{-3}	10^{-6}	1.66×10^{-24}	$1.604 \times 10^{-5} T^{-1}$	$1.219 \times 10^{-2} T^{-1}$	2.453×10^{-9}	$1.203 \times 10^{-4} T^{-1}$
1 $\text{dm}^3 \text{ mol}^{-1} \text{ s}^{-1} =$	10^3	1	10^{-3}	1.66×10^{-21}	$1.604 \times 10^{-2} T^{-1}$	$12.19 T^{-1}$	2.453×10^{-6}	$1.203 \times 10^{-1} T^{-1}$
1 $\text{m}^3 \text{ mol}^{-1} \text{ s}^{-1} =$	10^6	10^3	1	1.66×10^{-18}	$16.04 T^{-1}$	$1.219 \times 10^4 T^{-1}$	2.453×10^{-3}	$120.3 T^{-1}$
1 $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1} =$	6.023×10^{23}	6.023×10^{20}	6.023×10^{17}	1	$9.658 \times 10^{18} T^{-1}$	$7.34 \times 10^{21} T^{-1}$	1.478×10^{15}	$7.244 \times 10^{19} T^{-1}$
1 $(\text{mm Hg})^{-1} \text{ s}^{-1} =$	$6.236 \times 10^4 T$	$62.36 T$	$6.236 \times 10^{-2} T$	$1.035 \times 10^{-19} T$	1	760	4.56×10^{-2}	7.500
1 $\text{atm}^{-1} \text{ s}^{-1}$	$82.06 T$	$8.206 \times 10^{-2} T$	$8.206 \times 10^{-5} T$	$1.362 \times 10^{-22} T$	1.316×10^{-3}	1	6×10^{-5}	9.869×10^{-3}
1 $\text{ppm}^{-1} \text{ min}^{-1} =$ at 298 K, 1 atm total pressure	4.077×10^8	4.077×10^5	407.7	6.76×10^{-16}	21.93	1.667×10^4	1	164.5
1 $\text{m}^2 \text{ kN}^{-1} \text{ s}^{-1} =$	$8314 T$	$8.314 T$	$8.314 \times 10^{-3} T$	$1.38 \times 10^{-20} T$	0.1333	101.325	6.079×10^{-3}	1

To convert a rate constant from one set of units A to a new set B find the conversion factor for the row A under column B and multiply the old value by it, e.g. to convert $\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$ to $\text{m}^3 \text{ mol}^{-1} \text{ s}^{-1}$ multiply by 6.023×10^{17} .

Table adapted from High Temperature Reaction Rate Data No. 5, The University, Leeds (1970).

Equivalent third order rate constants

A \ B	$\text{cm}^6 \text{ mol}^{-2} \text{ s}^{-1}$	$\text{dm}^6 \text{ mol}^{-2} \text{ s}^{-1}$	$\text{m}^6 \text{ mol}^{-2} \text{ s}^{-1}$	$\text{cm}^6 \text{ molecule}^{-2} \text{ s}^{-1}$	$(\text{mm Hg})^{-2} \text{ s}^{-1}$	$\text{atm}^{-2} \text{ s}^{-1}$	$\text{ppm}^{-2} \text{ min}^{-1}$	$\text{m}^4 \text{ kN}^{-2} \text{ s}^{-1}$
1 $\text{cm}^6 \text{ mol}^{-2} \text{ s}^{-1} =$	1	10^{-6}	10^{-12}	2.76×10^{-48}	$2.57 \times 10^{-10} T^{-2}$	$1.48 \times 10^{-4} T^{-2}$	1.003×10^{-19}	$1.447 \times 10^{-8} T^{-2}$
1 $\text{dm}^6 \text{ mol}^{-2} \text{ s}^{-1} =$	10^6	1	10^{-6}	2.76×10^{-42}	$2.57 \times 10^{-4} T^{-2}$	$148 T^{-2}$	1.003×10^{-13}	$1.447 \times 10^{-2} T^{-2}$
1 $\text{m}^6 \text{ mol}^{-2} \text{ s}^{-1} =$	10^{12}	10^6	1	2.76×10^{-36}	$257 T^{-2}$	$1.48 \times 10^8 T^{-2}$	1.003×10^{-7}	$1.447 \times 10^4 T^{-2}$
1 $\text{cm}^6 \text{ molecule}^{-2} \text{ s}^{-1} =$	3.628×10^{47}	3.628×10^{41}	3.628×10^{35}	1	$9.328 \times 10^{37} T^{-2}$	$5.388 \times 10^{43} T^{-2}$	3.64×10^{28}	$5.248 \times 10^{39} T^{-2}$
1 $(\text{mm Hg})^{-2} \text{ s}^{-1} =$	$3.89 \times 10^9 T^2$	$3.89 \times 10^3 T^2$	$3.89 \times 10^{-3} T^2$	$1.07 \times 10^{-38} T^2$	1	5.776×10^5	3.46×10^{-5}	56.25
1 $\text{atm}^{-2} \text{ s}^{-1} =$	$6.733 \times 10^3 T^2$	$6.733 \times 10^{-3} T^2$	$6.733 \times 10^{-9} T^2$	$1.86 \times 10^{-44} T^2$	1.73×10^{-6}	1	6×10^{-11}	9.74×10^{-5}
1 $\text{ppm}^{-2} \text{ min}^{-1} =$ at 298 K, 1 atm total pressure	9.97×10^{18}	9.97×10^{12}	9.97×10^6	2.75×10^{-29}	2.89×10^4	1.667×10^{10}	1	1.623×10^8
1 $\text{m}^4 \text{ kN}^{-2} \text{ s}^{-1} =$	$6.91 \times 10^7 T^2$	$69.1 T^2$	$6.91 \times 10^{-5} T^2$	$1.904 \times 10^{-40} T^2$	0.0178	1.027×10^4	6.16×10^{-7}	1

See note to table for second order rate constants.

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11. ABSTRACT <i>(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)</i> <p>Chemical kinetics data for reactions of importance in combustion chemistry are compiled. Experimental, theoretical, evaluated, or estimated rate constants are given for reactions of O, O₂, O₃, H, H₂, OH, HO₂, H₂O, H₂O₂, N, N₂, N₃, NO, NO₂, NO₃, N₂O, N₂O₅, NH, NH₂, NH₃, NH=NH, NH₂=NH, NH₂=NH₂, HN₃, HNO, HONO, HONO₂, HO₂NO₂, NH₂O, NH₂O₂, S, S₂, SO, SO₂, SH, H₂S, and the aliphatic, alicyclic, and heterocyclic saturated and unsaturated C₁ to C₁₅ hydrocarbons, alcohols, aldehydes, ketones, thiols, ethers, peroxides, amines, amides, and their free radicals. The data were taken from the literature published between 1971 and 1982. Data previously issued in 1981 as NBSIR-81-2254, which covered the literature published from 1971 through 1977, are included. The data are reported as rate constants or in terms of the parameters <i>A</i>, <i>n</i>, and <i>B</i> of the extended Arrhenius expression $k = A(T/298)^n \times \exp(-B/T)$, where $B = E/R$. Data are given for 1931 reactions.</p>			
12. KEY WORDS <i>(Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)</i> Arrhenius parameters; carbon; chemical kinetics; combustion; compilation; free radicals; gas phase; hydrocarbons; hydrogen; nitrogen; oxygen; rate of reaction; sulfur.			
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